Electronic Supplementary Material for PCCP

Labile Ligands on some Lewis Super Acids: a Computational Study – Supplementary Materials

Paola Nava, Yannick Carissan and Stéphane Humbel
E-mail: paola.nava@univ-cezanne.fr
Aix-Marseille Université
Institut des Sciences Moléculaires de Marseille ISM2-UMR-CNRS-6263
Campus St. Jérôme, case D42 – 13397 Marseille cedex 20 – France

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We report the list of the compounds, for which the coordinates in format xyz (angstrom) are available in this document. We report, as well, energies computed at levels TPSS//TPSS (TPSS), B3LYP//TPSS, and B3LYP//B3LYP (B3LYP). The basis set is of def2-TZVP quality + diffuse functions on O, F, Cl (see the section 'Computational Details' of the article for more information).

OTCl = $ClSO_3^-$
OTf = $CF_3SO_3^-$
[1] = 1,6-diene, see Figure 1 in the article.

Table 1: Mechanism applied to the model system, 51 atoms, charge +1

Compound	TPSS	B3LYP//TPSS	B3LYP
Sn(OTCl)4	-4551.324311319	-4550.303302	-4550.305936
Sn(OTCl)4(C2H4)	-4629.956340612	-4628.867895	
Sn(OTCl)4((Me)2C=C(Me)2)	-4787.300360211	-4786.073763	-4786.076343165
Sn(OTCl)4(CH3Cl)	-5051.498757866	-5050.370287	-5050.3728978
Sn(OTCl)4(OC(CH3)2)	-4744.614313	-4743.457884	-4743.460456

Compound	TPSS	B3LYP//TPSS	B3LYP
Sn(OTCl)4(H2O)	-4627.821039	-4626.764350	-4626.766871
Sn(OTCl)4(MeOH)	-4667.144106	-4666.049888	-4666.052767
Sn(OTCl)4(CH3NO2)	-4796.498480636	-4795.318545	-4795.32341088
Sn(OTCl)4(HCOOCH3)	-4780.548785258	-4779.384089	-4779.38695338
Sn(OTCl)4((MeOOC)2CMe2)	-5126.561445620	-5125.157331	-5125.16076922
Sn(OTCl)4[1] (eta 1)	-5438.754971083	-5437.078788	-5437.08345858
Sn(OTCl)4[1] (eta 2)	-5438.770642577	-5437.098535	-5437.10271872
Sn(OTCl)4(DMSO)	-5104.709137763	-5103.512857	-5103.51584958
Sn(OTCl)4(DMSO)	-5104.705256552		
Sn(OTf)4	-4061.581627456	-4060.246851	-4060.2507436
Sn(OTf)4(C2H4)	-4140.210160795	-4138.808844	-4138.8125031
Sn(OTf)4((Me)2C=C(Me)2)	-4297.557032552	-4296.017422	-4296.0216068
Sn(OTf)4(CH3Cl)	-4561.756859749	-4560.314656	-4560.3186331
Sn(OTf)4(OC(CH3)2)	-4254.872571	-4253.402730	-4253.406578
Sn(OTf)4(H2O)	-4138.077979	-4136.707721	-4136.711954
Sn(OTf)4(MeOH)	-4177.400633458	-4175.993219	-4175.99725422
Sn(OTf)4(CH3NO2)	-4306.753701794	-4305.261969	-4305.2670133
Sn(OTf)4(HCOOCH3)	-4290.807581835	-4289.328966	-4289.3333173
Sn(OTf)4((MeOOC)2CMe2)	-4636.822236242	-4635.105454	
Sn(OTf)4[1] (eta 1)	-4949.014638644	-4947.023516	
Sn(OTf)4[1] (eta 2)	-4949.031081843	-4947.046258	
Sn(OTf)4(DMSO)	-4614.966221999	-4613.457384	-4613.46163385
Sn(OTCl)4(DMSO)2	-4549.689056109	-5103.512857	
Sn(OTCl)4(DMSO)3	-5103.050136668	-5656.713508	
Sn(OTCl)4(DMSO)4	-5656.408684940	-6209.867179	
Sn(OTCl)4(DMSO)4	-6209.754681500	-6763.057246	
Sn(OTCl)4(DMSO)5	-6763.099116080	-7316.226704	
Sn(OTCl)4(DMSO)6	-5658.089845733	-7869.390763	
Sn(OTf)4(DMSO)2	-4614.966222	-4613.457384	
Sn(OTf)4(DMSO)3	-5168.350059	-5166.661068	
Sn(OTf)4(DMSO)4	-5721.690641	-5719.812686	
Sn(OTf)4(DMSO)4	-6275.063020	-6273.004875	
Sn(OTf)4(DMSO)5	-6828.411394	-6826.170822	
Sn(OTf)4(DMSO)6	-7381.760990	-7379.333968	
In(OTCl)3(DMSO)2	-6211.434894543	-4548.573829	
In(OTCl)3(DMSO)3	-6764.804075735	-5101.754581	
In(OTCl)3(DMSO)4	-6764.791740516	-5654.927710	

Compound	TPSS	B3LYP//TPSS	B3LYP
In(OTCl)3(DMSO)5	-7318.155194057	-6208.087038	
In(OTCl)3(DMSO)6	-7871.505574357	-6761.249523	
In(OTf)3(DMSO)2	-4182.382130	-4181.032967	
In(OTf)3(DMSO)3	-4735.743350	-4734.213785	
In(OTf)3(DMSO)4	-5289.102797	-5287.388742	
In(OTf)3(DMSO)5	-5842.443564	-5840.542459	
In(OTf)3(DMSO)6	-6395.789486	-6393.705717	

Sn(OTCl)4

TPSS

21

Energy = -4551.324311319

Sn	-0.1297984	0.0214635	-0.1062365
O	0.6837507	-1.0036558	-1.8387326
O	-1.4782567	1.7548370	0.3824819
O	-1.9216259	-1.1058072	-0.3540201
O	1.2343099	1.1780982	0.8137796
S	-2.2034618	-1.3710987	1.1353318
S	2.8056259	1.1540523	0.6585239
O	-2.4254521	-2.7350193	1.4943866
O	3.2745399	2.4862326	0.9022812
O	-1.0875176	-0.6202004	1.8120697
O	3.1767093	0.4103990	-0.5170263
Cl	-3.9067448	-0.3442915	1.5293468
Cl	3.3372601	0.0212575	2.2944468
S	1.2832495	-2.1964307	-1.1034097
S	-1.4217048	2.3611655	-0.9962153
O	2.6141418	-2.5828724	-1.4360997
O	-2.6535493	2.7037341	-1.6334149
O	0.9682767	-1.8557371	0.3406259
O	-0.5179408	1.3800462	-1.7404722
Cl	0.0610548	-3.7606841	-1.5644529
Cl	-0.3171204	4.0545654	-0.8171227

B3LYP

21

Energy = -4550.305936

Sn	-0.140447	0.010612	-0.123000
O	0.733846	-0.973628	-1.833068
O	-1.563700	1.707420	0.371906
O	-1.875312	-1.193575	-0.320669
O	1.181659	1.204665	0.780162
S	-2.134142	-1.463376	1.160093
S	2.740998	1.276525	0.680273
O	-2.282834	-2.824466	1.523259
O	3.126687	2.624802	0.914921
O	-1.051704	-0.664193	1.806264
O	3.188422	0.550782	-0.465642
Cl	-3.872611	-0.520018	1.566511
Cl	3.285026	0.198819	2.338594
S	1.390534	-2.135054	-1.119150
S	-1.555068	2.293064	-0.999729
O	2.730826	-2.438891	-1.451315
O	-2.798537	2.561385	-1.625527
O	1.054334	-1.823212	0.310548
O	-0.623629	1.344940	-1.731551
Cl	0.259851	-3.751154	-1.603823
Cl	-0.531989	4.032508	-0.867641

Sn(OTCl)4(C2H4)

TPSS

27

Energy = -4629.956340612

Sn	-0.0292996	0.0434065	0.1893212
O	1.9108252	0.1204731	0.8328448
S	3.3144577	-0.0206989	0.1293284
O	4.2267883	0.8227731	0.8494651

B3LYP

27

Energy = -4628.870382190

Sn	-0.0273244	0.0486969	0.1885876
O	1.9082787	0.0362142	0.8104614
S	3.3094514	-0.0570933	0.1279528
O	4.1954006	0.7955611	0.8482906

O	3.1955870	0.0221283	-1.3004738	O	3.1980757	0.0019124	-1.2912483
Cl	3.7902026	-1.9681945	0.6445942	Cl	3.8290057	-1.9891557	0.6188464
O	-1.9667673	0.1080305	-0.4754728	O	-1.9637735	0.1701975	-0.4270901
S	-3.3946994	-0.1278531	0.1034280	S	-3.3986695	-0.0947656	0.0803147
O	-4.2767325	-0.3646408	-1.0015477	O	-4.2319164	-0.3589569	-1.0415055
O	-3.3708680	-1.0002970	1.2496127	O	-3.3960155	-0.9579793	1.2206112
Cl	-3.8489208	1.7681543	0.8259688	Cl	-3.9198216	1.7830197	0.7745390
O	-0.1710118	2.2327025	0.6205333	O	-0.1033365	2.2395836	0.6311565
S	0.1221801	2.6763030	-0.8017351	S	0.1793741	2.6896940	-0.7776777
O	-0.7841075	3.6011001	-1.4035604	O	-0.7175301	3.6193670	-1.3597593
O	0.3560741	1.3594010	-1.5128618	O	0.3781000	1.3784058	-1.4858978
Cl	1.9473042	3.5705718	-0.7112089	Cl	2.0102740	3.5533994	-0.7090288
O	0.3538438	-1.4599583	-1.3630852	O	0.3039370	-1.4690475	-1.3513549
S	0.0441455	-2.6833951	-0.5251492	S	0.0032394	-2.6812540	-0.5158166
O	0.9669582	-3.7717497	-0.5679723	O	0.9341842	-3.7487113	-0.5411485
O	-0.2497851	-2.0737302	0.8372546	O	-0.2951966	-2.0595384	0.8258867
Cl	-1.7421884	-3.3699310	-1.2093192	Cl	-1.7666754	-3.3886843	-1.1972438
C	-0.9212383	0.2033796	2.6839290	C	-0.9553410	0.2355405	2.7233173
C	0.3866195	0.2430586	3.0324330	C	0.3487658	0.1865290	3.0540847
H	-1.4792961	-0.7282745	2.6779003	H	-1.5686850	-0.6558348	2.6968860
H	0.9403486	-0.6639996	3.2567998	H	0.8459674	-0.7550447	3.2522074
H	0.9302371	1.1799538	3.1066406	H	0.9477184	1.0835998	3.1480042
H	-1.4867835	1.1202393	2.5328015	H	-1.4607819	1.1858053	2.5967717

Sn(OTCl)4(Me2C=CMe2)

TPSS				B3LYP			
39				39			
Energy = -4787.300360211				Energy = -4786.076343165			
C	-0.7161840	0.0448292	2.8595396	C	-0.7090719	0.0279939	2.8581826
C	0.6587684	0.2995291	2.9082845	C	0.6691566	0.2328798	2.9265574
C	1.2175064	1.6873512	3.0367711	C	1.2765223	1.5935645	3.0714514
Sn	-0.0137742	0.0025402	0.1218656	Sn	-0.0159700	-0.0085938	0.1266938
O	0.2090556	1.2859698	-1.7011281	O	0.1820797	1.2985738	-1.6576284
S	-0.0814649	2.6035604	-1.0412090	S	-0.0738790	2.6160276	-1.0032514
Cl	1.6950730	3.6163599	-1.0203717	Cl	1.7004566	3.6120828	-1.0412373
O	0.4013300	-1.4435604	-1.5284700	O	0.3456911	-1.4434117	-1.5249379
S	0.2082176	-2.7077690	-0.7346274	S	0.2005659	-2.7172949	-0.7554202
Cl	-1.5626608	-3.4950840	-1.3674333	Cl	-1.5501669	-3.5398616	-1.3732283
O	-0.0707986	-2.1827936	0.6646232	O	-0.0632520	-2.2182988	0.6389254
O	2.0136326	0.2100779	0.4269937	O	2.0120378	0.1215771	0.4140398
S	3.3451815	0.1645903	-0.3911387	S	3.3494127	0.1945969	-0.3614844
O	4.2652869	1.0559394	0.2657842	O	4.2221106	1.0572124	0.3710185
O	-1.9499592	-0.1211483	-0.5849611	O	-1.9755193	-0.1249283	-0.4698881
S	-3.4518862	-0.2728439	-0.2496105	S	-3.4806799	-0.2436769	-0.2127305
O	-4.1168333	-0.8129095	-1.4013261	O	-4.0972352	-0.8797907	-1.3280946

O	-0.3131184	2.2130369	0.4091596	O	-0.2681337	2.2259655	0.4361130
O	1.1918874	-3.7381591	-0.8505449	O	1.2085376	-3.7041911	-0.9059862
C	1.6503930	-0.8007028	3.1883077	C	1.6204340	-0.8963293	3.2043327
O	3.1298872	0.2077550	-1.8083268	O	3.1564710	0.3504930	-1.7634201
Cl	3.9944106	-1.7587083	0.0608633	Cl	4.0601227	-1.7252425	-0.0636923
O	-3.6646983	-0.8414725	1.0594117	O	-3.7567541	-0.6940851	1.1193141
Cl	-4.0412116	1.7142291	-0.1124791	Cl	-4.0562065	1.7399137	-0.2729203
O	-1.0494099	3.4662408	-1.6422287	O	-1.0466381	3.4705934	-1.5820284
C	-1.2664235	-1.3198026	3.1922444	C	-1.3138715	-1.3160112	3.1638977
C	-1.7376168	1.1543230	2.9669928	C	-1.6897650	1.1676934	2.9824387
H	2.6673532	-0.4726432	2.9717803	H	2.6425506	-0.6123877	2.9677608
H	1.5908821	-1.0427798	4.2604623	H	1.5741447	-1.1155147	4.2787503
H	1.4500775	-1.7203215	2.6366980	H	1.3807981	-1.8155845	2.6773777
H	2.1375407	1.7970858	2.4578576	H	2.2052465	1.6704900	2.5070019
H	0.5189683	2.4778984	2.7712135	H	0.6196147	2.4122083	2.8017057
H	1.4928282	1.8145818	4.0959837	H	1.5447065	1.7063964	4.1303947
H	-0.5369026	-2.1231375	3.1207227	H	-0.6299841	-2.1503407	3.0659954
H	-1.6159087	-1.2640841	4.2347922	H	-1.6547591	-1.2747905	4.2062823
H	-2.1391852	-1.5591891	2.5826377	H	-2.1986970	-1.4996594	2.5587062
H	-1.8528154	1.3887325	4.0358454	H	-1.8045126	1.3867732	4.0510663
H	-1.4577314	2.0729323	2.4539991	H	-1.3822157	2.0831480	2.4892950
H	-2.7099370	0.8194541	2.6034285	H	-2.6682441	0.8739300	2.6105042

Sn(OTCl)4(CH3Cl)

TPSS				B3LYP			
26				26			
Energy = -5051.498757866				Energy= -5050.3728978			
Sn	0.2141683	0.3719143	-0.5238986	Sn	0.005694	0.141120	-0.146529
O	2.1648394	-0.1698888	-0.3363793	O	2.000524	0.368580	0.076702
S	2.9275772	-1.2908960	0.4435228	S	3.117020	-0.221648	0.975330
O	2.0546849	-1.9821045	1.3593020	O	2.571848	-1.125996	1.940850
O	4.1840474	-0.7494399	0.8737766	O	3.987679	0.833202	1.368640
Cl	3.3383449	-2.6061366	-1.0901810	Cl	4.136214	-1.361288	-0.394308
O	-1.6283435	1.1686472	-0.8868807	O	-1.984982	0.123217	-0.525122
S	-2.9687120	1.2091187	-0.0846622	S	-3.268253	-0.289225	0.237044
O	-4.0246107	1.4585703	-1.0217744	O	-4.269664	-0.612407	-0.719944
O	-3.0479736	0.1269547	0.8648843	O	-2.962295	-1.180804	1.313943
Cl	-2.7277297	2.9417884	1.0190788	Cl	-3.814863	1.501367	1.093678
O	0.8532051	2.3646236	0.2325385	O	-0.171744	2.295000	0.398454
S	1.2222030	2.9262039	-1.1272629	S	-0.006511	2.824012	-0.998884
O	0.6821753	4.2001478	-1.4809935	O	-0.972503	3.748525	-1.468087
O	0.9269017	1.7603846	-2.0513306	O	0.178188	1.555747	-1.788331
Cl	3.2477130	3.0988066	-1.1071162	Cl	1.795839	3.746457	-1.023563
O	-0.0124870	-0.8248883	-2.3744043	O	0.292225	-1.220975	-1.860149
S	-0.6398325	-2.0310466	-1.7177876	S	0.192009	-2.505973	-1.096439

O	-0.1233638	-3.3216513	-2.0425584	O	1.197164	-3.483061	-1.301270
O	-0.6313341	-1.6372071	-0.2447512	O	-0.000997	-2.008205	0.316655
Cl	-2.5977091	-1.9984202	-2.2652066	Cl	-1.583346	-3.324804	-1.623228
Cl	-0.0511243	0.3989608	2.1429972	Cl	-0.322631	0.301305	2.509890
C	-0.7522064	-1.1699427	2.7721508	C	-0.368809	-1.355704	3.273810
H	-0.8248079	-1.0094578	3.8466348	H	-0.482553	-1.156583	4.334922
H	-1.7234493	-1.2799540	2.2986619	H	-1.228190	-1.863757	2.854240
H	-0.0414480	-1.9483339	2.5097480	H	0.576497	-1.830288	3.040960

Sn(OTCl)4(H2O)

TPSS				B3LYP			
24				24			
Energy = -4627.821038973				Energy = -4626.76687100			
Sn	0.0717531	0.0900549	-0.1629432	Sn	0.043278	0.022013	0.023993
O	0.8819481	-0.8541061	-1.9517142	O	0.379152	-1.249548	-1.701728
O	-1.2722509	1.8194195	0.4923700	O	-0.581257	2.176357	0.594143
O	-1.6589967	-0.9991235	-0.5050409	O	-1.956414	-0.422952	-0.137887
O	1.5292325	1.3859935	0.3871540	O	1.883524	0.723283	0.457790
S	-2.7099345	-1.6780650	0.3957405	S	-3.141407	-0.593283	0.816708
S	3.0966189	1.3110076	0.3278125	S	3.333381	0.193240	0.272524
O	-3.1898566	-2.8803568	-0.2121289	O	-3.988321	-1.645295	0.379574
O	3.5869694	2.6543551	0.4315975	O	4.208135	1.314700	0.241001
O	-2.2523306	-1.7241776	1.7857219	O	-2.683221	-0.586230	2.193319
O	3.5308104	0.4107228	-0.7051237	O	3.372389	-0.825116	-0.725276
Cl	-4.2444713	-0.3175560	0.3600526	Cl	-4.152880	1.160366	0.553160
Cl	3.5083109	0.3881351	2.1387609	Cl	3.632731	-0.738049	2.091686
S	1.4540664	-2.0862956	-1.2676724	S	0.552269	-2.555646	-0.965787
S	-1.3808571	2.4162714	-0.8878277	S	-0.544545	2.678800	-0.809176
O	2.7770958	-2.4916757	-1.6083981	O	1.641640	-3.383536	-1.322055
O	-2.6834210	2.7369371	-1.3794279	O	-1.667777	3.393503	-1.296654
O	1.1497212	-1.7931896	0.1938129	O	0.447274	-2.096244	0.466254
O	-0.5509707	1.4550930	-1.7274963	O	-0.152083	1.436981	-1.580247
Cl	0.2013614	-3.6081150	-1.7788585	Cl	-1.151047	-3.598160	-1.322980
Cl	-0.3005211	4.1381811	-0.8342142	Cl	1.066388	3.901778	-0.928232
O	-0.1846541	-0.2113265	1.9816961	O	-0.162038	-0.033881	2.188077
H	-0.3547283	0.6400952	2.4254391	H	0.113535	0.794454	2.608152
H	-1.0048951	-0.8022787	2.1006881	H	-1.118910	-0.221966	2.421613

Sn(OTCl)4(MeOH)

TPSS				B3LYP			
27				27			
Energy = -4667.144106098				Energy = -4666.05276677			
Sn	-0.0051241	0.0418046	0.1018358	Sn	-0.004574	0.025771	0.136899
O	0.3893338	-1.2029862	-1.6391356	O	0.465329	-1.305762	-1.481554
O	-0.6750682	2.1099797	0.6141071	O	-0.448960	2.174201	0.601798

O	-1.9909687	-0.4261325	-0.2712772	O	-1.996154	-0.221623	-0.321979
O	1.8505951	0.5835601	0.7246347	O	1.866356	0.244521	0.850330
S	-3.2639231	-0.5609481	0.5878551	S	-3.313490	-0.328286	0.449116
S	3.2818339	0.4126988	0.1057877	S	3.287491	0.355978	0.223348
O	-4.0944031	-1.6122752	0.0842105	O	-4.174486	-1.281271	-0.156966
O	4.0637803	1.5497952	0.4968707	O	4.059359	1.222145	1.049218
O	-2.9329183	-0.5442184	2.0130305	O	-3.054098	-0.422536	1.873508
O	3.2138506	-0.0431682	-1.2549067	O	3.210189	0.533641	-1.188886
Cl	-4.2244398	1.2100920	0.2165886	Cl	-4.131130	1.517958	0.148059
Cl	3.9744008	-1.1870870	1.2413713	Cl	3.988864	-1.553433	0.555842
S	0.5679180	-2.5319791	-0.9255854	S	0.347849	-2.644823	-0.786701
S	-0.4797151	2.6789167	-0.7726170	S	-0.226715	2.680062	-0.791079
O	1.7121093	-3.3145248	-1.2659504	O	1.409181	-3.561503	-0.991473
O	-1.5499647	3.4333598	-1.3443228	O	-1.240374	3.478028	-1.379512
O	0.3846964	-2.1384635	0.5238741	O	0.018826	-2.239501	0.609796
O	0.0076161	1.4682679	-1.5515369	O	0.158890	1.415711	-1.517530
Cl	-1.0852155	-3.6194221	-1.4051053	Cl	-1.339092	-3.480510	-1.541038
Cl	1.1360115	3.9065914	-0.6328589	Cl	1.464686	3.790552	-0.708372
O	-0.4057383	-0.0439705	2.2210894	O	-0.515050	-0.023130	2.223017
H	-1.3952167	-0.2235197	2.3215734	H	-1.498279	-0.179752	2.292020
C	0.3694771	-0.8184158	3.1958470	C	0.211309	-0.715851	3.278827
H	0.1034190	-0.4339799	4.1820260	H	-0.258584	-0.443196	4.221657
H	0.1350851	-1.8794513	3.1029177	H	0.172538	-1.790918	3.118388
H	1.4195379	-0.6316996	2.9821720	H	1.234350	-0.357487	3.250619

Sn(OTCl)4(OC(CH3)2)

TPSS				B3LYP			
31				31			
Energy = -4744.614313059				Energy = -4743.46045619			
Sn	0.2242716	0.1034340	-1.1443096	Sn	0.013821	0.133969	-0.227198
O	2.1656730	-0.4992650	-0.9720906	O	2.023099	0.332901	-0.067713
S	2.9902945	-1.2339376	0.1244032	S	3.118949	-0.029629	0.954894
O	2.2384066	-1.3743848	1.3497800	O	2.553885	-0.628653	2.128534
O	4.3174984	-0.6899841	0.1342412	O	4.031822	1.056756	1.065638
Cl	3.1256085	-3.1244940	-0.6927716	Cl	4.094493	-1.532367	-0.052521
O	-1.6276129	0.8457386	-1.5986402	O	-1.983950	0.066187	-0.595598
S	-2.8842603	1.1771576	-0.7445468	S	-3.245223	-0.279650	0.219984
O	-4.0188392	1.2250706	-1.6193946	O	-4.277702	-0.669925	-0.677098
O	-2.9165886	0.4062899	0.4763441	O	-2.921936	-1.088354	1.359095
Cl	-2.4880479	3.1318528	-0.1740467	Cl	-3.767734	1.572894	0.962824
O	0.9780067	2.1877327	-0.9506577	O	-0.159767	2.296817	0.289848
S	1.2790391	2.3874265	-2.4200553	S	-0.024329	2.817196	-1.109776
O	0.7717110	3.5681038	-3.0457679	O	-0.998241	3.741172	-1.567539
O	0.8842137	1.0530886	-3.0172767	O	0.149987	1.547998	-1.895442
Cl	3.3125047	2.4555984	-2.5508700	Cl	1.778851	3.747287	-1.176321

O	-0.1189707	-1.4071030	-2.7781942	O	0.298711	-1.125973	-2.061464
S	-0.7003768	-2.4734468	-1.8936463	S	0.257150	-2.452262	-1.381126
O	-0.2123568	-3.8100209	-2.0226368	O	1.281178	-3.390268	-1.668265
O	-0.6053530	-1.8388429	-0.5110511	O	0.081719	-2.055640	0.064568
Cl	-2.6971311	-2.5143046	-2.3102661	Cl	-1.511596	-3.296789	-1.914371
O	0.0706582	0.6271080	0.9497839	O	-0.288723	0.203191	1.893408
C	-0.2594619	0.2048193	2.0817517	C	-0.391683	-0.461678	2.938397
C	-0.0805256	1.1510255	3.2233847	C	-0.674036	0.290486	4.191335
H	-1.0521933	1.2956708	3.7131341	H	-1.581821	-0.114871	4.647770
H	0.5780390	0.6810157	3.9651909	H	0.141405	0.106997	4.897882
H	0.3292751	2.1048290	2.8934944	H	-0.782170	1.354890	4.003190
C	-0.8035194	-1.1550349	2.3492033	C	-0.254054	-1.938671	3.003018
H	-0.0642524	-1.8984353	2.0331756	H	0.696476	-2.234909	2.559542
H	-1.0330134	-1.2808430	3.4079654	H	-0.318450	-2.293459	4.028656
H	-1.7026969	-1.3058648	1.7443699	H	-1.051494	-2.385484	2.405595

Sn(OTCl)4(CH3NO2)

TPSS

28

Energy = -4796.498480636

Sn	0.0266533	0.0982149	-0.0880273
O	1.8029625	0.0912904	0.8845143
S	3.2845324	-0.0520914	0.3749024
O	4.1143849	0.6957741	1.2761714
O	3.3634710	0.1070352	-1.0511300
Cl	3.6288954	-2.0510870	0.7806300
O	-1.9118466	0.2237941	-0.7306739
S	-3.2993949	-0.0720294	-0.0898270
O	-4.2371353	-0.2942953	-1.1512524
O	-3.2021663	-0.9910085	1.0194936
Cl	-3.7659924	1.7758595	0.7346220
O	-0.1455865	2.2639240	0.4757705
S	0.2619343	2.7876799	-0.8800102
O	-0.5764249	3.7614550	-1.5043236
O	0.5343715	1.5087605	-1.6574039
Cl	2.0912280	3.6373525	-0.6044801
O	0.5172500	-1.2354938	-1.7473022
S	0.0944866	-2.5357683	-1.0875564
O	0.9886078	-3.6449755	-1.1796150
O	-0.3154541	-2.0745961	0.2947003
Cl	-1.6350207	-3.0683530	-2.0217353
O	-0.7972348	0.2206651	2.0053559
N	-0.6948492	-0.6110704	2.9618949
O	0.1246196	-1.4875774	3.0374408
C	-1.7361941	-0.4223715	4.0242163

B3LYP

28

Energy=-4795.32341088

Sn	0.049328	0.101851	-0.093189
O	1.823223	-0.009319	0.848598
S	3.305947	-0.073271	0.373138
O	4.096516	0.641632	1.317850
O	3.401133	0.176055	-1.028044
Cl	3.706552	-2.071370	0.660695
O	-1.878810	0.255043	-0.720519
S	-3.282979	0.009833	-0.133359
O	-4.183554	-0.250586	-1.203135
O	-3.236173	-0.857394	1.007333
Cl	-3.748105	1.886950	0.591132
O	-0.057476	2.261106	0.483606
S	0.338924	2.795374	-0.859281
O	-0.493377	3.774703	-1.457506
O	0.576639	1.526050	-1.637845
Cl	2.171586	3.618926	-0.600562
O	0.512396	-1.238816	-1.738225
S	0.079745	-2.534681	-1.101898
O	0.973986	-3.630855	-1.182243
O	-0.348033	-2.078257	0.260029
Cl	-1.623744	-3.062011	-2.067972
O	-0.755396	0.201338	1.995834
N	-0.729155	-0.645381	2.926883
O	0.051762	-1.539219	3.015267
C	-1.798471	-0.450962	3.944979

H	-1.4623243	-1.0624461	4.8589585	H	-1.602939	-1.139811	4.758688
H	-1.7513857	0.6372813	4.2780140	H	-1.769364	0.591323	4.252546
H	-2.6807376	-0.7132060	3.5579072	H	-2.734981	-0.661014	3.428581

Sn(OTCl)4(HCOOCH3)

TPSS				B3LYP			
29				29			
Energy = -4780.548785258				Energy = -4779.38695338			
Sn	0.3322408	0.4485476	-1.0794337	Sn	0.024814	0.096359	-0.307158
O	2.2621030	-0.1669133	-0.8571808	O	2.027983	0.296355	-0.076881
S	2.9756366	-1.0979201	0.1701778	S	3.048385	-0.051157	1.029499
O	2.0804426	-1.5120844	1.2257763	O	2.397442	-0.620737	2.173677
O	4.2596740	-0.5349829	0.4748204	O	3.956003	1.034868	1.182754
Cl	3.3124034	-2.7631455	-0.9967133	Cl	4.082518	-1.576111	0.125709
O	-1.5304479	1.2076391	-1.4618310	O	-1.972703	-0.009975	-0.673888
S	-2.8151122	1.3056751	-0.5896861	S	-3.210629	-0.344081	0.183170
O	-3.9374062	1.4839780	-1.4627646	O	-4.255878	-0.786973	-0.673089
O	-2.8310286	0.3055400	0.4519727	O	-2.848555	-1.095257	1.349281
Cl	-2.5159619	3.1266533	0.3688349	Cl	-3.751265	1.534824	0.856812
O	1.0227563	2.4927945	-0.5111305	O	-0.153539	2.306944	0.004638
S	1.3955639	2.9200909	-1.9120203	S	0.017802	2.681898	-1.434824
O	0.8994309	4.1754765	-2.3807682	O	-0.939290	3.554231	-2.012391
O	1.0550771	1.6874838	-2.7290774	O	0.204171	1.335904	-2.084765
Cl	3.4303205	3.0240352	-1.9254223	Cl	1.827809	3.590476	-1.556783
O	0.0844106	-0.8206014	-2.8815117	O	0.325863	-1.369997	-1.929118
S	-0.5206188	-2.0188477	-2.1909117	S	0.271056	-2.620320	-1.104773
O	0.0082969	-3.3087720	-2.5008415	O	1.297137	-3.580262	-1.291336
O	-0.5061989	-1.5936641	-0.7343013	O	0.083385	-2.069082	0.280377
Cl	-2.4867476	-2.0209652	-2.7242351	Cl	-1.492142	-3.507654	-1.573924
O	0.0599453	0.5830830	1.0517346	O	-0.309653	0.334075	1.790061
C	-0.3980183	-0.2853177	1.8283353	C	-0.373740	-0.525286	2.685384
H	-0.7437432	-1.2671607	1.5110944	H	-0.286735	-1.592385	2.502968
O	-0.4979922	-0.0776521	3.1019730	O	-0.553253	-0.217942	3.919338
C	-0.0476960	1.2261905	3.6179811	C	-0.673648	1.190505	4.281804
H	-0.2511189	1.1741379	4.6845312	H	-0.814233	1.186147	5.356822
H	1.0179494	1.3342254	3.4139104	H	0.239931	1.710898	4.004279
H	-0.6215794	2.0154825	3.1319175	H	-1.531669	1.621306	3.771403

Sn(OTCl)4((MeOOC)2CMe2)

TPSS				B3LYP			
44				44			
Energy = -5126.561445620				Energy = -5125.16076922			
Sn	-0.0009851	0.0013109	-0.4975474	Sn	0.001598	-0.009921	-0.545743
O	-1.4431475	1.4697991	-0.5586468	O	-1.327699	1.545341	-0.631912
S	-2.3803158	2.1243776	0.4734345	S	-2.192922	2.318134	0.360443

O	-2.6294340	1.2373078	1.5956385	O	-2.474283	1.514588	1.523486
O	-1.9884254	3.4828250	0.7345528	O	-1.702494	3.644706	0.546303
Cl	-4.1194533	2.1976105	-0.6158609	Cl	-3.939245	2.463066	-0.692549
O	-0.9691103	-1.0505037	-1.9420729	O	-1.032452	-1.014255	-1.959225
O	1.4411972	-1.4670090	-0.5587291	O	1.336480	-1.560365	-0.573823
O	0.9665845	1.0539601	-1.9418028	O	1.073573	0.976612	-1.944888
S	-2.2956586	-1.8562309	-1.9333639	S	-2.434344	-1.643674	-2.022199
S	2.3803143	-2.1200337	0.4725998	S	2.254840	-2.274468	0.415570
S	2.2954811	1.8558049	-1.9338184	S	2.466558	1.627511	-1.971896
O	-3.1995327	-1.3837109	-0.9131816	O	-3.295959	-1.097332	-1.017253
O	2.6412437	-1.2270837	1.5873485	O	2.576674	-1.416101	1.526683
O	3.1985544	1.3806877	-0.9141210	O	3.294551	1.126581	-0.916113
O	-2.7255558	-2.0329961	-3.2891165	O	-2.848325	-1.724142	-3.380150
O	1.9818782	-3.4743795	0.7455320	O	1.785670	-3.595150	0.684141
O	2.7251836	2.0315572	-3.2897633	O	2.934589	1.671559	-3.314088
Cl	-1.6209888	-3.7198661	-1.2821339	Cl	-2.015176	-3.586261	-1.420862
Cl	4.1119389	-2.2109112	-0.6270507	Cl	3.953744	-2.454005	-0.706217
Cl	1.6260719	3.7212231	-1.2820940	Cl	1.993309	3.579146	-1.449815
O	0.8797899	1.0693008	1.1330746	O	0.920154	0.981367	1.101259
C	0.9710545	0.8148606	2.3584421	C	0.991772	0.728062	2.318640
C	0.0017216	-0.0014737	3.2087860	C	-0.043076	-0.023154	3.156303
O	1.9070868	1.3744557	3.0672653	O	1.957932	1.206737	3.025337
C	-0.7646398	1.0021537	4.1256725	C	-0.717968	1.014848	4.095075
C	0.7713451	-1.0089322	4.1189019	C	0.639929	-1.116611	4.026555
C	-0.9703067	-0.8148050	2.3587025	C	-1.080630	-0.732777	2.288268
C	2.9019159	2.2054379	2.3576476	C	3.024023	1.951991	2.350804
O	-1.9055106	-1.3749101	3.0682640	O	-2.079341	-1.186236	2.965844
O	-0.8813737	-1.0674066	1.1327857	O	-0.979740	-0.987756	1.072937
H	3.6023587	2.4935431	3.1376986	H	3.739585	2.166370	3.136741
H	3.3675859	1.6024366	1.5796947	H	3.450410	1.332629	1.567404
H	2.3930779	3.0685365	1.9278423	H	2.608174	2.864995	1.931629
C	-2.9015204	-2.2049272	2.3592445	C	-3.144574	-1.903236	2.260893
H	-3.6010210	-2.4935618	3.1399487	H	-3.885521	-2.103208	3.026879
H	-3.3681383	-1.6012381	1.5823962	H	-3.536331	-1.271604	1.469171
H	-2.3934878	-3.0677710	1.9279680	H	-2.740553	-2.824178	1.847752
H	-1.4741494	0.4421667	4.7369498	H	-1.462851	0.508795	4.704968
H	-0.0397983	1.4935898	4.7775865	H	0.041148	1.439360	4.748973
H	-1.3095976	1.7455330	3.5432594	H	-1.208774	1.807765	3.536086
H	0.0487682	-1.5023328	4.7718614	H	-0.112444	-1.567642	4.670927
H	1.3136873	-1.7506019	3.5318758	H	1.114364	-1.884897	3.420947
H	1.4835614	-0.4515065	4.7293675	H	1.400575	-0.649440	4.647990

Sn(OTCl)4[1] (eta 1)
TPSS
64

B3LYP
64

Energy = -5438.754971083

Sn	0.6221338	0.6313095	2.8686424
O	2.4208857	1.2313547	2.1103729
S	2.8980043	2.6241192	1.5953846
O	4.0122474	2.4113137	0.7146872
O	1.7807767	3.4430507	1.1914802
Cl	3.6610781	3.4576209	3.3221347
O	-1.1328167	-0.1354918	3.5647889
S	-2.2621868	-0.9197299	2.8245952
O	-3.0965051	-0.0106014	2.0763094
O	-1.7553438	-2.1139273	2.2019966
Cl	-3.3296324	-1.4874637	4.4865376
O	0.5170585	0.9106965	-3.6202570
C	0.4460925	1.0974585	-2.4273413
C	-0.4701824	0.2719912	-1.4921904
O	1.1678938	2.0019949	-1.7426396
C	0.1885008	-1.1388302	-1.3211694
C	-1.8645324	0.1339644	-2.2033843
C	-0.6201853	1.0074090	-0.1699011
C	2.1235454	2.7751297	-2.5271416
O	-1.3598224	2.0733131	-0.2294564
O	-0.0870466	0.5696110	0.8891713
H	2.5920219	3.4470872	-1.8114439
H	2.8554467	2.0991581	-2.9724677
H	1.5945312	3.3239038	-3.3086012
C	-1.6017953	2.8957492	0.9650689
H	-2.2586220	3.6863749	0.6096007
H	-2.1015231	2.2879526	1.7189265
H	-0.6510803	3.2994957	1.3120642
H	-0.0509032	-1.6840701	-2.2367019
C	1.6728597	-1.1382242	-1.0770377
H	-0.3384626	-1.6445399	-0.5036313
C	-2.8314935	-0.7674688	-1.4927725
H	-2.2913600	1.1391548	-2.3030920
H	-1.6338467	-0.2173524	-3.2108301
H	2.0003404	-0.7001144	-0.1366174
H	-3.1531322	-0.4312727	-0.5064792
C	-3.3622403	-1.9136728	-1.9517505
C	2.6254914	-1.6428108	-1.8801760
C	4.0747156	-1.5888492	-1.4623126
H	4.4937951	-2.6012271	-1.3845903
H	4.6769957	-1.0581763	-2.2119368
H	4.2011019	-1.0870559	-0.4993870
C	2.3822935	-2.3023590	-3.2130903
H	2.7396041	-3.3406590	-3.1920362

Energy = -5437.08345858

Sn	1.159381	-0.000073	0.360731
O	1.060160	-2.011833	0.613070
S	1.164135	-3.198288	-0.369737
O	0.471077	-4.312415	0.186257
O	0.899655	-2.775005	-1.712459
Cl	3.169279	-3.638339	-0.264354
O	1.161458	2.023800	0.241849
S	0.044772	3.067478	0.016044
O	-0.449272	2.985596	-1.326476
O	-0.873173	3.085456	1.109628
Cl	1.187106	4.760422	0.137565
O	-4.613619	-2.282599	-1.363371
C	-3.480307	-1.897502	-1.274619
C	-3.110140	-0.434996	-0.938941
O	-2.397405	-2.667171	-1.408621
C	-3.363236	-0.223269	0.588900
C	-4.048095	0.494570	-1.776896
C	-1.655174	-0.200649	-1.327336
C	-2.622380	-4.075971	-1.640346
O	-1.449830	-0.115713	-2.594367
O	-0.756850	-0.075730	-0.460598
H	-1.633829	-4.520199	-1.685209
H	-3.197250	-4.496844	-0.817648
H	-3.161451	-4.216505	-2.575897
C	-0.123919	0.112739	-3.160124
H	-0.291932	0.146966	-4.231062
H	0.259194	1.066292	-2.807357
H	0.524200	-0.718814	-2.898883
H	-4.434917	-0.066822	0.689405
C	-2.906072	-1.327295	1.499509
H	-2.888623	0.719293	0.871478
C	-3.886436	1.959056	-1.497528
H	-3.859342	0.298029	-2.835594
H	-5.057504	0.146012	-1.574366
H	-1.833667	-1.469391	1.567466
H	-2.899143	2.367664	-1.696246
C	-4.820435	2.816212	-1.072638
C	-3.670778	-2.125269	2.252940
C	-3.040055	-3.161758	3.144653
H	-3.304594	-2.983774	4.192161
H	-3.406884	-4.163309	2.897918
H	-1.953590	-3.165899	3.061850
C	-5.172813	-2.087204	2.317605
H	-5.501825	-1.863822	3.337693

H	1.3328369	-2.3075334	-3.5131869	H	-5.624118	-1.358250	1.648534
H	2.9525408	-1.7900814	-3.9985820	H	-5.586936	-3.067945	2.065150
C	-4.3531427	-2.6819378	-1.1129162	C	-4.487831	4.272041	-0.883678
H	-4.5384804	-2.1898258	-0.1548205	H	-3.446632	4.484642	-1.123255
H	-5.3097788	-2.7886086	-1.6419815	H	-5.123353	4.900757	-1.516012
H	-3.9878083	-3.6984735	-0.9151756	H	-4.672348	4.581041	0.150214
C	-3.0580584	-2.5348319	-3.2908506	C	-6.246944	2.460201	-0.755392
H	-3.9791361	-2.6363464	-3.8799288	H	-6.930466	3.035421	-1.388103
H	-2.3401236	-1.9645031	-3.8842646	H	-6.478087	1.405352	-0.889975
H	-2.6615090	-3.5500604	-3.1569451	H	-6.484436	2.729544	0.278728
O	1.6642209	-0.1611034	4.6112997	O	2.599651	0.105955	1.982133
O	0.2409679	2.4515769	3.6567808	O	2.492488	-0.181767	-1.129374
S	2.0355943	-1.4882062	3.9741987	S	1.592381	0.138290	3.101813
Cl	0.9091800	-2.8783450	4.9315905	Cl	1.709410	1.996845	3.885961
O	1.4266215	-1.3652081	2.5843731	O	0.288133	0.099619	2.342895
O	3.3997490	-1.9017720	4.0538503	O	1.755512	-0.791840	4.157741
S	-0.7447376	2.8416508	4.8238098	S	3.512909	0.832828	-1.730432
Cl	0.1533380	4.6301038	5.3232203	Cl	4.843885	-0.524802	-2.506705
O	-2.0382221	3.1623050	4.2811444	O	2.917431	1.510525	-2.837288
O	-0.5987535	1.9558838	5.9450585	O	4.186392	1.551088	-0.699660

Sn(OTCl)4[1] (eta 2)

TPSS				B3LYP			
64				64			
Energy = -5438.770642577				Energy = -5437.10271872			
Sn	-0.0784937	0.2287659	-3.2716068	Sn	1.371538	0.005978	0.088463
O	-1.2911945	1.8947244	-3.2647801	O	1.442402	-1.737935	1.162473
S	-1.8762621	2.7590183	-2.1316522	S	0.432014	-2.747919	1.698292
O	-2.4815228	1.9370525	-1.1020340	O	-0.778336	-2.087073	2.113899
O	-0.9665989	3.8033267	-1.7334417	O	0.328884	-3.887610	0.844251
Cl	-3.4094069	3.6485043	-3.1674190	Cl	1.395406	-3.350336	3.399481
O	-1.3067403	-0.6576925	-4.6288459	O	2.580949	0.897567	1.440692
O	1.1073211	-1.4465501	-3.4551278	O	1.451010	1.764629	-0.962454
O	0.9423946	1.1189355	-4.7899688	O	2.965207	-0.690048	-0.942148
S	-2.7794319	-1.1385901	-4.5516633	S	2.461345	1.231775	2.935919
S	1.8858601	-2.3282749	-2.4642562	S	0.495705	2.613430	-1.793593
S	2.4135165	1.5883363	-4.9322216	S	3.221038	-1.063850	-2.410899
O	-3.5099521	-0.4679787	-3.5046621	O	1.410349	0.482301	3.556046
O	2.3988300	-1.5450067	-1.3544200	O	-0.488671	1.789060	-2.446595
O	3.2832513	0.9249250	-3.9919335	O	2.257912	-0.456126	-3.279162
O	-3.2969402	-1.2292734	-5.8855435	O	3.762153	1.285036	3.509110
O	1.1838185	-3.5519426	-2.1834410	O	0.050461	3.758586	-1.065445
O	2.7360574	1.6572031	-6.3273461	O	4.614606	-0.968204	-2.679867
Cl	-2.5131746	-3.1030321	-3.8947795	Cl	1.784180	3.192574	2.841524
Cl	3.5019841	-2.8188409	-3.6353251	Cl	1.770752	3.282142	-3.246969

Cl	2.2571230	3.5618991	-4.2699433	Cl	2.766364	-3.088535	-2.382899
O	1.0940080	1.1162666	-1.7279667	O	-0.070223	-0.887370	-1.191524
C	1.2275336	0.8478261	-0.5058164	C	-1.290510	-0.693426	-1.374259
C	0.1647883	0.2935500	0.4339995	C	-2.308568	-0.271583	-0.316973
O	2.3387951	1.1590954	0.0953450	O	-1.812136	-0.952145	-2.524276
C	-0.3926394	1.5051917	1.3131079	C	-3.153914	-1.556087	0.076234
C	0.8334358	-0.8164520	1.3613231	C	-3.220564	0.878578	-0.918937
C	-0.9825104	-0.3366008	-0.3425626	C	-1.611678	0.280049	0.923914
C	3.4295605	1.7228221	-0.7253293	C	-0.936325	-1.368626	-3.621871
O	-1.9921377	-0.6578667	0.4075281	O	-2.393725	0.430509	1.933483
O	-0.9920182	-0.6582693	-1.5625449	O	-0.426910	0.679031	0.990124
H	4.2475525	1.8448733	-0.0192439	H	-1.598859	-1.449998	-4.476477
H	3.6676120	1.0176335	-1.5198111	H	-0.169930	-0.614443	-3.771137
H	3.1012915	2.6765957	-1.1387326	H	-0.485448	-2.326704	-3.375163
C	-3.1504218	-1.3087820	-0.2339227	C	-1.854562	0.985374	3.174471
H	-3.8607832	-1.4328965	0.5799374	H	-2.695338	0.978178	3.859087
H	-3.5260979	-0.6543804	-1.0191137	H	-1.040804	0.355712	3.521154
H	-2.8318798	-2.2667545	-0.6450356	H	-1.500123	1.996518	2.990813
H	-1.3382192	1.1588609	1.7293670	H	-3.618983	-1.331053	1.030106
C	0.5271199	1.9952476	2.3921017	C	-4.175490	-2.011574	-0.923010
H	-0.6358311	2.3199106	0.6222919	H	-2.442765	-2.360441	0.277111
C	-0.0680086	-1.4731440	2.3586476	C	-4.305930	1.398896	-0.030098
H	1.3283975	-1.5409073	0.7142435	H	-2.570978	1.673577	-1.274955
H	1.6145157	-0.2625227	1.8942397	H	-3.674555	0.426439	-1.802317
H	1.5059949	2.3429561	2.0676108	H	-3.805792	-2.224486	-1.919538
H	-0.5565564	-0.8047642	3.0659279	H	-5.023208	0.660066	0.310639
C	-0.2606862	-2.7949927	2.5172370	C	-4.526247	2.673915	0.310590
C	0.2338752	2.1270701	3.6981240	C	-5.469201	-2.260489	-0.690799
C	1.2484593	2.7169183	4.6460293	C	-6.349707	-2.795552	-1.788367
H	0.8538480	3.6240157	5.1224144	H	-6.776486	-3.763274	-1.506481
H	1.4786367	2.0119457	5.4558190	H	-7.194499	-2.123601	-1.970167
H	2.1800632	2.9737342	4.1343884	H	-5.805393	-2.923071	-2.724048
C	-1.0784560	1.7589044	4.3401548	C	-6.172189	-2.078852	0.626186
H	-1.5522609	2.6536500	4.7647524	H	-6.540382	-3.042836	0.991113
H	-1.7915527	1.3008505	3.6512138	H	-5.547543	-1.649352	1.406914
H	-0.9132208	1.0676975	5.1768180	H	-7.051812	-1.439644	0.502792
C	-1.1288717	-3.3021445	3.6421999	C	-5.731229	3.038628	1.136537
H	-1.5465096	-2.4837163	4.2354437	H	-6.326604	2.164555	1.401142
H	-1.9570815	-3.9084263	3.2514615	H	-5.432080	3.545249	2.059747
H	-0.5540696	-3.9562488	4.3111555	H	-6.374015	3.739580	0.594573
C	0.3456862	-3.8736905	1.6581440	C	-3.666009	3.843977	-0.078628
H	-0.4400841	-4.5329617	1.2671233	H	-3.373400	4.410699	0.810645
H	0.9202078	-3.4973683	0.8104177	H	-2.757981	3.577547	-0.614439
H	1.0080765	-4.5082359	2.2619233	H	-4.234241	4.536544	-0.707899

Sn(OTCl)4(DMSO)

TPSS (1)

31

Energy = -5104.709137763

Sn	0.0327285	0.4038225	-0.2454412
O	1.8170404	-0.6234802	-0.3767200
S	2.9216914	-0.9557563	0.6590715
O	2.4826282	-0.6452772	2.0042062
O	4.1988103	-0.5024113	0.1911155
Cl	2.9406796	-3.0199198	0.5124624
O	-1.6465854	1.5894207	-0.2432966
S	-3.1011521	1.2525338	0.1786139
O	-4.0051900	2.0682488	-0.5778775
O	-3.2995035	-0.1710298	0.3092675
Cl	-3.1330547	2.0184123	2.1256467
O	1.0605355	2.1214343	0.6461726
S	1.3259007	2.8323307	-0.6717697
O	0.9074372	4.1930051	-0.7798379
O	0.7791713	1.8463610	-1.6903175
Cl	3.3403366	2.7818749	-0.9130942
O	-0.6614283	-0.7105379	-1.8091426
S	-0.7967536	-2.2610678	-1.7799733
O	0.0261372	-2.8681172	-2.7833603
O	-0.7468625	-2.7264341	-0.4053123
Cl	-2.7466634	-2.4604941	-2.4068951
O	-0.5472996	-0.2750953	1.6050485
S	-0.2857301	-1.6741197	2.2984920
C	-1.9597499	-2.3049651	2.5143691
H	-2.3187844	-2.5718549	1.5206417
H	-1.8811916	-3.1946048	3.1467650
H	-2.5837682	-1.5345192	2.9699813
C	0.0675822	-1.1417781	3.9824582
H	1.0445438	-0.6593807	3.9527969
H	-0.7160125	-0.4581139	4.3145809
H	0.1044196	-2.0421104	4.6027219

B3LYP (1)

31

Energy = -5103.51584958

Sn	0.064814	0.425112	-0.277005
O	1.813690	-0.643862	-0.368808
S	2.935207	-0.990863	0.621220
O	2.486967	-0.818197	1.976296
O	4.173516	-0.425316	0.205757
Cl	3.072602	-3.019464	0.306008
O	-1.594015	1.620946	-0.279446
S	-3.052103	1.355532	0.126289
O	-3.917206	2.177654	-0.647280
O	-3.301834	-0.047314	0.275656
Cl	-3.077725	2.148732	2.050854
O	1.127681	2.114050	0.621559
S	1.415706	2.827677	-0.675776
O	1.008020	4.180391	-0.779277
O	0.865378	1.855844	-1.689429
Cl	3.420671	2.762012	-0.903300
O	-0.649157	-0.698848	-1.804260
S	-0.864090	-2.225890	-1.838375
O	-0.056171	-2.831788	-2.839257
O	-0.861762	-2.741981	-0.493881
Cl	-2.800935	-2.307069	-2.503369
O	-0.537847	-0.286392	1.537759
S	-0.366105	-1.677702	2.247255
C	-2.065760	-2.217858	2.440427
H	-2.428059	-2.467906	1.446676
H	-2.045756	-3.107444	3.072019
H	-2.659420	-1.420879	2.883519
C	0.004356	-1.156401	3.922967
H	1.004987	-0.731777	3.901189
H	-0.735851	-0.427446	4.248734
H	-0.012507	-2.047752	4.551547

TPSS (2)

31

Energy = -5104.705256552

Sn	-0.0301166	0.1356727	-0.1441614
O	1.8320527	-0.0955810	0.6915011
S	3.3062154	-0.2004176	0.1827209
O	4.1476723	0.3764773	1.1969478
O	3.4258493	0.1610781	-1.2015364
Cl	3.5977770	-2.2532537	0.2980688

O	-1.9614971	0.3830282	-0.7796556
S	-3.3407340	0.1200959	-0.1096499
O	-4.3372810	0.1191503	-1.1412162
O	-3.2801713	-0.9409755	0.8655344
Cl	-3.6163616	1.8770778	0.9711388
O	-0.0117811	2.3225484	0.4277916
S	0.3670173	2.8154653	-0.9442710
O	-0.4382321	3.8306849	-1.5474640
O	0.5462595	1.5226098	-1.7227140
Cl	2.2501425	3.5774235	-0.7426529
O	0.3639807	-1.1774164	-1.8438661
S	-0.0844521	-2.4957080	-1.2370894
O	0.7683063	-3.6258827	-1.4322497
O	-0.4403152	-2.1082970	0.1718345
Cl	-1.8584472	-2.9174048	-2.1563660
O	-0.6015824	0.1520407	1.8814155
S	-0.1363214	-0.9430765	2.9036696
C	-1.6600906	-1.2608035	3.8107171
H	-2.3462681	-1.7186910	3.0959457
H	-1.4229172	-1.9527528	4.6237417
H	-2.0627828	-0.3174986	4.1848742
C	0.7858424	0.0218357	4.1164098
H	1.7089083	0.3338715	3.6238430
H	0.1882290	0.8828798	4.4226156
H	1.0109839	-0.6346475	4.9618387

Sn(OTf)4

TPSS			
33			
Energy = -4061.581627456			
Sn	0.0201048	-0.0912816	-0.1561558
S	1.7073671	1.9785992	-1.1000437
O	0.8004668	1.0099118	-1.8589275
O	1.5473388	1.4779950	0.3223448
O	1.5834031	3.3769302	-1.3623789
C	3.4638727	1.5116576	-1.6301405
F	4.3252765	2.2071284	-0.8821889
F	3.6809404	0.2047520	-1.4738834
F	3.6109054	1.8423416	-2.9168873
S	-1.6562952	-2.1359403	-1.1522944
O	-1.0228376	-0.9311151	-1.8528571
O	-1.3804837	-3.4280381	-1.7034263
O	-1.3116666	-1.8692687	0.2898437
C	-3.5193773	-1.8561975	-1.3049903
F	-4.1409024	-2.7775692	-0.5617700

B3LYP			
33			
Energy = -4060.2507436			
Sn	-0.075771	0.076200	-0.155045
S	-0.720373	-2.518024	-1.096566
O	-0.308686	-1.262326	-1.839004
O	-0.788378	-2.001729	0.312431
O	-0.016996	-3.719053	-1.359201
C	-2.496668	-2.831754	-1.625845
F	-2.984604	-3.814211	-0.881107
F	-3.231292	-1.740214	-1.469797
F	-2.491919	-3.190836	-2.902617
S	0.645436	2.628325	-1.147387
O	0.559551	1.271882	-1.825104
O	-0.100457	3.686683	-1.730591
O	0.391702	2.263202	0.276678
C	2.457961	3.105808	-1.255407
F	2.636097	4.212159	-0.545157

F	-3.8401072	-0.6359130	-0.8802695	F	3.212810	2.132179	-0.776254
F	-3.8655291	-1.9999997	-2.5875073	F	2.758362	3.331465	-2.527161
S	1.9519464	-1.5370075	1.2480999	S	-2.453831	0.608864	1.218106
O	1.6208421	-1.5097378	-0.2556180	O	-2.114770	0.685812	-0.268916
O	0.7897524	-0.7779665	1.8372647	O	-1.103390	0.389985	1.818922
O	3.2837973	-1.1705031	1.6204755	O	-3.520628	-0.252556	1.583370
C	1.7410294	-3.3494290	1.7597247	C	-2.994885	2.349514	1.689077
F	1.8945749	-3.4158158	3.0855147	F	-3.185285	2.369275	3.001204
F	0.5424467	-3.8112246	1.4165048	F	-2.079272	3.237836	1.350030
F	2.6959297	-4.0619859	1.1551618	F	-4.133734	2.607313	1.061035
S	-2.0920563	2.3293960	0.4338944	S	2.866598	-1.192923	0.464343
O	-1.4741683	0.9055762	0.7414996	O	1.675113	-0.218481	0.758076
O	-3.5235307	2.2186000	0.4480364	O	4.089164	-0.466045	0.536570
O	-1.3788398	2.9643708	-0.6460951	O	2.547813	-2.033411	-0.648395
C	-1.6132760	3.2077055	2.0322841	C	2.784879	-2.246446	2.011428
F	-2.1741959	2.5949021	3.0827535	F	3.003959	-1.497630	3.087500
F	-0.2816050	3.2152169	2.1839645	F	1.591552	-2.825678	2.113452
F	-2.0587164	4.4694126	1.9631493	F	3.725020	-3.182132	1.922443

Sn(OTf)4(C2H4)
TPSS B3LYP
39 39

Energy = -4140.210160795				Energy = -4138.812503098			
C	-0.6614442	0.0057704	2.7239992	C	-0.7143184	0.0355755	2.7765219
C	0.6666597	0.0935847	2.9678312	C	0.6100254	0.0641306	3.0156566
Sn	-0.0132571	0.0295001	0.1533044	Sn	-0.0121434	0.0242065	0.1730377
O	0.1836770	-2.1214770	0.7237568	O	0.0988769	-2.1310812	0.7307152
S	0.5974104	-2.6069295	-0.6609241	S	0.5119274	-2.6326308	-0.6335401
C	-0.7425171	-3.8205395	-1.2150928	C	-0.8591951	-3.7788780	-1.2083559
O	1.9458478	0.4131916	0.6101233	O	1.9520625	0.2764997	0.6374830
S	3.3529227	0.3870933	-0.1073972	S	3.3472543	0.3589758	-0.0658815
C	4.2494650	-0.7256223	1.1227397	C	4.2662466	-0.8451320	1.0360414
O	-2.0262784	-0.0949046	-0.2079304	O	-2.0166473	-0.0527883	-0.1771949
S	-3.3367855	-0.7537764	0.3376434	S	-3.3506323	-0.6739410	0.3138529
C	-4.2645433	0.7856024	0.9031444	C	-4.2472950	0.8755863	0.8581250
O	-0.4469803	2.1859591	0.6616491	O	-0.3785078	2.2000017	0.6647755
S	-0.5589590	2.6320489	-0.7849982	S	-0.4725720	2.6470711	-0.7689806
C	0.7311892	3.9959694	-1.0021495	C	0.8480649	3.9617621	-0.9920535
O	-0.0105383	1.4247823	-1.5310189	O	0.0345708	1.4273605	-1.4980112
O	0.3906982	-1.3571004	-1.4970348	O	0.3769115	-1.3812329	-1.4585048
O	3.9759213	1.6753325	0.0349534	O	3.9398312	1.6303117	0.1952806
O	3.2990696	-0.3015504	-1.3683367	O	3.3036550	-0.1959379	-1.3799723
O	-4.0951716	-1.2719536	-0.7666904	O	-4.0865675	-1.1728931	-0.7993277
O	-3.0876055	-1.5447530	1.5201638	O	-3.1533370	-1.4668643	1.4914274
O	-1.8018226	3.1855965	-1.2280866	O	-1.6909352	3.2267480	-1.2112340

O	1.8349314	-3.3141413	-0.7751946	O	1.7137663	-3.3804950	-0.7258599
H	-1.1698155	-0.9534972	2.6702118	H	-1.2645576	-0.8961771	2.7290677
H	1.2869143	-0.7946994	3.0459950	H	1.1875117	-0.8475638	3.1050680
H	1.1610845	1.0512837	3.0987210	H	1.1465755	0.9961785	3.1403358
H	-1.2823690	0.8966107	2.7121978	H	-1.2916740	0.9511877	2.7563200
F	5.5067832	-0.8985287	0.6991209	F	5.5261055	-0.9145847	0.6211951
F	4.2697886	-0.1458684	2.3387237	F	4.2428379	-0.4124197	2.3007952
F	3.6489536	-1.9205389	1.2297632	F	3.7152409	-2.0541180	0.9866663
F	-5.4260973	0.3947978	1.4472081	F	-5.4304192	0.5200130	1.3506195
F	-3.5534488	1.4533814	1.8367902	F	-3.5506664	1.5019597	1.8165965
F	-4.5062605	1.6006925	-0.1246960	F	-4.4197486	1.7009728	-0.1628622
F	0.8070857	4.2984292	-2.3014061	F	0.9206510	4.2617515	-2.2813893
F	0.3174337	5.0659960	-0.3120875	F	0.4786933	5.0329595	-0.2985554
F	1.9187611	3.6008467	-0.5541337	F	2.0147237	3.5240138	-0.5585299
F	-0.4407197	-4.2321812	-2.4494553	F	-0.5648558	-4.1878553	-2.4342943
F	-0.7339190	-4.8612223	-0.3748851	F	-0.9027422	-4.8165543	-0.3823080
F	-1.9402653	-3.2418182	-1.2099873	F	-2.0207900	-3.1495792	-1.2079761

Sn(OTf)4(Me2C=CMe2)

TPSS				B3LYP			
51				51			
Energy = -4297.557032552				Energy = -4296.021606816			
C	1.4682880	1.2818509	3.2712929	C	1.4775049	1.2711768	3.2613796
C	0.6973146	0.0070346	3.0696451	C	0.6968242	0.0069437	3.0605997
C	1.5310094	-1.2371901	3.2611451	C	1.5175174	-1.2389375	3.2611225
C	-0.6994974	-0.0294999	3.0697080	C	-0.6977173	-0.0190041	3.0625633
C	-1.5321365	1.2137900	3.2673623	C	-1.5181835	1.2260720	3.2646148
C	-1.4729703	-1.3045053	3.2591498	C	-1.4797396	-1.2834521	3.2563059
O	2.0283572	-0.3774343	0.3369370	O	2.0310461	-0.3328910	0.3362273
S	3.3760923	0.2529343	-0.1438902	S	3.3820269	0.2415468	-0.1552991
C	4.3880601	-1.3354967	-0.2529133	C	4.3705888	-1.3484628	-0.2008471
Sn	-0.0028944	-0.0006475	0.3320433	Sn	-0.0004986	0.0001060	0.3110558
O	0.1380008	2.2383168	0.7730268	O	0.1092175	2.3010278	0.7590521
S	-0.0641497	2.6654045	-0.6684321	S	-0.0570319	2.6915157	-0.6759150
O	-1.2217625	3.4515430	-0.9766076	O	-1.1956950	3.4616434	-1.0382208
O	0.1305791	1.3633832	-1.4156435	O	0.1435024	1.3770926	-1.3834604
O	-0.1358244	-1.3645595	-1.4184549	O	-0.1392289	-1.3783680	-1.3857786
S	0.0626033	-2.6660918	-0.6714980	S	0.0574968	-2.6913222	-0.6751992
O	1.2246100	-3.4471246	-0.9768824	O	1.1985813	-3.4620197	-1.0287290
O	-0.1473431	-2.2399265	0.7694507	O	-0.1172788	-2.2984957	0.7583601
O	-2.0315511	0.3669081	0.3507022	O	-2.0316618	0.3314753	0.3337508
S	-3.3785368	-0.2423318	-0.1592641	S	-3.3844903	-0.2375357	-0.1588272
C	-4.3843661	1.3509859	-0.2440667	C	-4.3707472	1.3540340	-0.1981209
C	1.4276382	3.7725488	-1.0895218	C	1.4332673	3.7638466	-1.1025234
C	-1.4192288	-3.7813212	-1.0927217	C	-1.4289320	-3.7659877	-1.1073555

O	3.9714691	1.0146163	0.9310872	O	3.9772247	1.0342497	0.8812069
O	3.2926467	0.7856469	-1.4781389	O	3.3107256	0.7211851	-1.4982170
O	-3.2834117	-0.7422519	-1.5056844	O	-3.3150517	-0.7115878	-1.5037871
O	-3.9881088	-1.0259684	0.8905778	O	-3.9809213	-1.0324364	0.8753737
H	2.5602983	-1.0630796	2.9442677	H	2.5428817	-1.0816006	2.9357196
H	1.5510138	-1.4618758	4.3380544	H	1.5440555	-1.4442650	4.3384390
H	1.1468120	-2.1150246	2.7438325	H	1.1226868	-2.1196640	2.7662048
H	2.3344841	1.3336816	2.6036507	H	2.3560643	1.3015465	2.6149499
H	0.8731131	2.1863111	3.1708055	H	0.9045965	2.1815477	3.1325971
H	1.8744133	1.2459375	4.2937270	H	1.8600428	1.2478637	4.2896183
H	-0.8680896	-2.2071349	3.2053747	H	-0.8911054	-2.1911935	3.1962243
H	-1.9335108	-1.2502319	4.2564806	H	-1.9339618	-1.2291477	4.2529657
H	-2.3007649	-1.3763080	2.5453731	H	-2.3105360	-1.3476188	2.5512553
H	-1.5652379	1.4170846	4.3481666	H	-1.5589558	1.4180736	4.3440115
H	-1.1340302	2.0982142	2.7728823	H	-1.1162173	2.1118698	2.7850566
H	-2.5564045	1.0486103	2.9307797	H	-2.5396809	1.0741749	2.9242706
F	-5.6590394	1.0117620	-0.4959145	F	-5.6318195	1.0444110	-0.4943497
F	-4.3335329	2.0062536	0.9295197	F	-4.3402795	1.9481847	0.9988182
F	-3.9419681	2.1491504	-1.2173807	F	-3.8940204	2.1839955	-1.1133560
F	-1.0946616	-5.0306248	-0.7340051	F	-1.1531993	-5.0063193	-0.7138402
F	-2.5092923	-3.4034333	-0.4284771	F	-2.5157071	-3.3415115	-0.4861559
F	-1.6360654	-3.7342449	-2.4082242	F	-1.6065946	-3.7415040	-2.4194541
F	5.6667614	-0.9888790	-0.4709500	F	5.6327968	-1.0360230	-0.4886402
F	4.3146696	-2.0243636	0.9004607	F	4.3344106	-1.9511898	0.9916667
F	3.9639708	-2.1059270	-1.2565187	F	3.8987137	-2.1722203	-1.1242741
F	1.0833431	5.0345908	-0.8023773	F	1.1499280	5.0087242	-0.7292980
F	2.4933938	3.4338971	-0.3671101	F	2.5118524	3.3495797	-0.4603591
F	1.6944018	3.6663382	-2.3919213	F	1.6292670	3.7224668	-2.4113832

Sn(OTf)4(CH3Cl)

TPSS				B3LYP			
38				38			
Energy = -4561.756859749				Energy = -4560.31863310			
Sn	-0.0014885	0.2090047	-0.2763949	Sn	0.066300	-0.035259	-0.087227
O	1.8034305	-0.7205517	-0.3027684	O	-1.928149	0.180266	0.135398
S	2.6363738	-1.4923067	0.7824270	S	-2.892126	0.453877	1.325167
O	1.8335068	-2.4920766	1.4489217	O	-2.415889	1.536578	2.135238
O	3.4703888	-0.5930976	1.5353402	O	-3.325163	-0.767410	1.924050
O	-1.7392121	1.2606070	-0.4056726	O	2.033814	-0.361294	-0.417824
S	-3.0958721	1.2923310	0.3824842	S	3.388574	-0.051602	0.278804
O	-4.1720364	1.4464323	-0.5558123	O	4.340172	0.353871	-0.700527
O	-3.1343668	0.2829044	1.4150433	O	3.191254	0.704019	1.481070
O	0.9735516	2.0459012	0.5315003	O	-0.132314	-2.221864	0.355114
S	1.1736765	2.7086131	-0.8202768	S	-0.237359	-2.656948	-1.080031
O	0.6253289	4.0158308	-1.0147337	O	0.687445	-3.622488	-1.556675

O	0.7539883	1.6067583	-1.7786932	O	-0.305237	-1.330962	-1.794893
O	-0.4287395	-0.8693067	-2.1580579	O	-0.051069	1.441392	-1.719965
S	-0.9539195	-2.1333746	-1.5111821	S	0.069129	2.673098	-0.868876
O	-0.3051157	-3.3741167	-1.8041754	O	-0.973906	3.634032	-0.919265
O	-1.0603482	-1.7182863	-0.0477668	O	0.413654	2.077348	0.475361
Cl	-0.0750536	0.0913896	2.4018819	Cl	0.333947	-0.359504	2.565191
C	-0.8708864	-1.4537757	2.9745107	C	0.621981	1.241604	3.392608
H	-0.8108316	-1.3901668	4.0598183	H	0.691832	0.987441	4.445756
H	-1.8928392	-1.4218664	2.6076726	H	1.553396	1.628772	2.997710
H	-0.2765229	-2.2688364	2.5703883	H	-0.239251	1.862030	3.175251
C	-2.9248093	2.9550067	1.2515010	C	3.880233	-1.779806	0.801957
C	3.0455822	2.8730054	-1.0348566	C	-1.947474	-3.411529	-1.263636
C	3.7571939	-2.4090861	-0.4260624	C	-4.326880	1.113961	0.317254
C	-2.7378055	-2.3058457	-2.1100417	C	1.629224	3.543061	-1.445975
F	-4.0115833	3.1383141	2.0162892	F	5.046663	-1.705031	1.437939
F	-2.8384715	3.9445268	0.3573307	F	4.001590	-2.568109	-0.258060
F	-1.8320047	2.9697007	2.0345925	F	2.964086	-2.289508	1.627605
F	3.6406237	1.6873020	-0.9269192	F	-2.876812	-2.555990	-0.874017
F	3.5044061	3.7019696	-0.0915930	F	-1.998610	-4.508105	-0.518562
F	3.2808437	3.3912930	-2.2451607	F	-2.127052	-3.724818	-2.540737
F	3.0375036	-3.1918464	-1.2373482	F	-3.957212	2.188995	-0.368860
F	4.5963088	-3.1684566	0.2945915	F	-5.301244	1.440479	1.162934
F	4.4673469	-1.5409320	-1.1593496	F	-4.766490	0.181268	-0.522843
F	-3.4074077	-1.1709303	-1.9194521	F	2.652009	2.705248	-1.442185
F	-2.7128118	-2.6074068	-3.4115235	F	1.419728	3.998307	-2.673559
F	-3.3179280	-3.2986246	-1.4264527	F	1.869015	4.556133	-0.622605

Sn(OTf)4(OC(CH3)2)

TPSS				B3LYP			
43				43			
Energy = -4254.872571452				Energy = -4253.40657846			
Sn	-0.0095245	0.0460975	-0.7308484	Sn	0.068555	0.012521	-0.123099
O	1.7550099	-0.9550511	-0.5299210	O	-1.928569	0.285399	0.073570
S	2.6345081	-1.2833770	0.7195826	S	-2.905054	0.294083	1.275068
O	1.8774972	-1.9970627	1.7257466	O	-2.479453	1.226043	2.281301
O	3.4657073	-0.1699218	1.0981600	O	-3.294191	-1.028718	1.648004
O	-1.7249293	1.0893034	-1.0953258	O	2.050387	-0.291602	-0.420715
S	-3.0069451	1.4321774	-0.2713663	S	3.357088	-0.129198	0.392282
O	-4.1516960	1.3773653	-1.1366434	O	4.380262	0.403177	-0.444045
O	-3.0086073	0.7728616	1.0164577	O	3.100924	0.432771	1.689025
O	1.0619454	1.9915012	-0.5161752	O	-0.179738	-2.185914	0.202454
S	1.2201121	2.2505800	-1.9998902	S	-0.235247	-2.568122	-1.246864
O	0.7103794	3.4796662	-2.5292151	O	0.689899	-3.536317	-1.721557
O	0.7245488	0.9503037	-2.6036052	O	-0.255646	-1.220531	-1.915192
O	-0.4637107	-1.4231986	-2.3557937	O	-0.051394	1.448502	-1.819082

S	-1.0495360	-2.4890827	-1.4630270	S	0.110056	2.708288	-1.025766
O	-0.4627766	-3.7950927	-1.4715326	O	-0.903138	3.700209	-1.112139
O	-1.1453863	-1.7675317	-0.1266431	O	0.447646	2.168298	0.339143
O	0.0015614	0.4976203	1.3884596	O	0.234747	-0.271259	1.998968
C	-0.3351342	0.0822956	2.5219133	C	0.403438	0.279459	3.101046
C	0.1044424	0.9022511	3.6899913	C	0.403663	-0.598525	4.302273
H	-0.7822721	1.2051706	4.2615048	H	1.333563	-0.440011	4.856110
H	0.7028365	0.2643424	4.3535360	H	-0.411511	-0.281569	4.960512
H	0.6786640	1.7728501	3.3756886	H	0.288141	-1.644705	4.033679
C	-1.1184304	-1.1602015	2.7634359	C	0.597198	1.740718	3.275677
H	-0.5308275	-2.0133949	2.4059488	H	-0.229875	2.272986	2.805111
H	-1.3393746	-1.2802244	3.8247299	H	0.664051	2.004649	4.328201
H	-2.0427448	-1.1265230	2.1800787	H	1.515197	2.031828	2.760908
C	3.7446139	-2.5508086	-0.1236721	C	-4.361305	1.076035	0.396948
C	-2.8373897	-2.7016631	-2.0295406	C	1.689307	3.501661	-1.652355
C	-2.6986785	3.2553922	0.0783318	C	3.790155	-1.925581	0.679374
C	3.0811810	2.2667632	-2.3219416	C	-1.945430	-3.286581	-1.527566
F	4.6196432	-3.0012179	0.7897317	F	-5.359089	1.178049	1.273184
F	4.4167665	-1.9871379	-1.1364499	F	-4.748112	0.317184	-0.624032
F	3.0222801	-3.5778309	-0.5863693	F	-4.039445	2.285819	-0.047379
F	3.6202860	3.2891086	-1.6472785	F	-2.063661	-4.387718	-0.795140
F	3.6409065	1.1222289	-1.9315526	F	-2.878850	-2.414238	-1.184362
F	3.2794398	2.4410021	-3.6342882	F	-2.065201	-3.589639	-2.815244
F	-2.5537956	3.9423438	-1.0583617	F	3.929791	-2.563168	-0.475111
F	-1.5925453	3.4056535	0.8310085	F	2.834382	-2.517968	1.398954
F	-3.7523403	3.7363491	0.7578482	F	4.936205	-1.975642	1.356311
F	-3.4578717	-1.5231771	-2.0762448	F	2.687719	2.634913	-1.613031
F	-3.4636629	-3.5088049	-1.1630605	F	1.968960	4.546892	-0.880287
F	-2.8341501	-3.2619253	-3.2434074	F	1.489207	3.906225	-2.900016

Sn(OTf)4(H2O)

TPSS				B3LYP			
36				36			
Energy = -4138.068488854				Energy = -4136.71195416			
Sn	0.0521704	-0.0249179	0.0259790	Sn	0.053063	0.001067	0.130902
O	0.1904378	-1.3786469	-1.6795502	O	0.472814	-1.279874	-1.568361
O	-0.1269997	2.2398713	0.5695024	O	-0.555503	2.227894	0.675003
O	-2.0239168	-0.0078665	0.0118301	O	-1.974261	-0.354544	0.023934
O	2.0090038	0.3948138	0.3446823	O	1.910302	0.576159	0.654519
S	-3.1177124	-0.2285544	1.0837323	S	-3.087433	-0.758546	1.000888
S	3.3963483	-0.2764480	0.0246824	S	3.359802	0.485179	0.080083
O	-4.0108012	-1.2935710	0.7358765	O	-3.718679	-1.975228	0.622743
O	4.3488907	0.7732567	-0.2095362	O	3.998057	1.750762	0.232582
O	-2.5416782	-0.1972032	2.4333591	O	-2.638397	-0.592666	2.374744
O	3.2481787	-1.3965870	-0.8660207	O	3.374874	-0.226457	-1.157815

S	0.1614044	-2.6847327	-0.8953437	S	0.692515	-2.573235	-0.818762
S	-0.1848445	2.6710599	-0.8690011	S	-0.694957	2.617677	-0.752207
O	1.1873023	-3.6532019	-1.1148109	O	1.912835	-3.268394	-1.011332
O	-1.2637220	3.5109808	-1.2948173	O	-1.935409	3.134864	-1.212292
O	-0.0465571	-2.1695444	0.5244680	O	0.325184	-2.156245	0.581745
O	-0.0244210	1.3453153	-1.6190094	O	-0.167870	1.386710	-1.473443
O	-0.0045714	0.0327334	2.2053114	O	-0.143197	-0.006976	2.286323
H	0.3282366	0.9010326	2.5006104	H	0.147511	0.823706	2.691009
H	-0.9849429	-0.0363005	2.4778851	H	-1.098649	-0.192924	2.540165
C	1.4493270	3.6277314	-1.2092382	C	0.593899	3.942010	-1.076048
C	3.7861265	-0.9771329	1.7258712	C	4.113421	-0.632484	1.378464
C	-1.4585303	-3.5245111	-1.4057918	C	-0.672316	-3.721733	-1.409701
C	-4.0836431	1.3783622	0.9165575	C	-4.323489	0.616339	0.708125
F	-5.1306882	1.3207484	1.7494786	F	-5.381883	0.386159	1.478367
F	-4.5160306	1.5243868	-0.3386738	F	-4.691169	0.628786	-0.565518
F	-3.3079820	2.4186634	1.2501901	F	-3.785384	1.787264	1.033028
F	1.1331146	4.8554038	-1.6247750	F	0.258194	5.019527	-0.375149
F	2.1625421	3.7041950	-0.0844354	F	1.790388	3.518789	-0.705962
F	2.1502793	2.9981161	-2.1519510	F	0.592136	4.227969	-2.370702
F	-2.4549815	-2.6441717	-1.4622315	F	-1.842170	-3.108061	-1.374107
F	-1.7380622	-4.4777435	-0.5115961	F	-0.691234	-4.785729	-0.617370
F	-1.2707650	-4.0730531	-2.6095762	F	-0.390718	-4.088424	-2.652592
F	3.7898090	0.0022536	2.6474876	F	4.034870	-0.058576	2.579677
F	2.8682693	-1.8944857	2.0734613	F	3.475297	-1.800659	1.414082
F	4.9940428	-1.5524991	1.6911215	F	5.389903	-0.835287	1.070896

Sn(OTf)4(MeOH)

TPSS				B3LYP			
39				39			
Energy = -4177.400633458				Energy = -4175.9972542			
Sn	0.0372544	0.0389519	0.1550595	Sn	0.021902	0.033033	0.146073
O	0.4859798	-1.2244064	-1.5561161	O	0.472622	-1.245159	-1.521736
O	-0.5827031	2.1502662	0.6431572	O	-0.598846	2.153961	0.631172
O	-1.9993192	-0.3368387	-0.0460840	O	-1.997636	-0.356536	-0.048540
O	1.9394342	0.4953354	0.6877334	O	1.921901	0.454011	0.669965
S	-3.1292050	-0.8227828	0.8889004	S	-3.150819	-0.792247	0.863545
S	3.3444615	0.5783997	-0.0218671	S	3.313681	0.618116	-0.017594
O	-3.7659489	-2.0110796	0.4012393	O	-3.786800	-1.976370	0.398398
O	3.9154550	1.8749652	0.2207749	O	3.845941	1.904506	0.290959
O	-2.7009763	-0.7716105	2.2918510	O	-2.747828	-0.708445	2.258852
O	3.3145907	-0.0123861	-1.3330012	O	3.296223	0.109106	-1.351016
S	0.6828087	-2.5487761	-0.8304447	S	0.681330	-2.570726	-0.820148
S	-0.7421785	2.5783507	-0.7977092	S	-0.730835	2.590483	-0.794995
O	1.9188441	-3.2439758	-1.0181633	O	1.915315	-3.239028	-1.032047
O	-2.0183433	3.0576623	-1.2360824	O	-1.987156	3.076089	-1.246506

O	0.2686652	-2.1905210	0.5804389	O	0.277858	-2.235915	0.579017
O	-0.1426366	1.3917900	-1.5444635	O	-0.140786	1.405821	-1.526946
O	-0.2463323	-0.0050884	2.2937414	O	-0.255945	-0.039340	2.272446
H	-1.2045298	-0.3014762	2.4479607	H	-1.208704	-0.288529	2.451507
C	0.6498123	-0.6556066	3.2557517	C	0.638395	-0.649042	3.246738
H	0.2163363	-0.4914018	4.2437193	H	0.199079	-0.485718	4.228757
H	0.7335203	-1.7201319	3.0326096	H	0.749298	-1.711694	3.042257
H	1.6121552	-0.1570601	3.1725685	H	1.591566	-0.137883	3.173261
C	0.4797368	3.9943443	-1.0574903	C	0.499116	3.987296	-1.031445
C	-4.3695230	0.5814710	0.6944185	C	-4.359599	0.613463	0.604842
C	-0.6672602	-3.6838330	-1.5192307	C	-0.649975	-3.696350	-1.517308
C	4.2780263	-0.6012072	1.1116672	C	4.277335	-0.591961	1.035667
F	0.0640398	5.0413433	-0.3353742	F	0.090557	5.022598	-0.307197
F	1.7011229	3.6336993	-0.6717750	F	1.703181	3.609430	-0.640248
F	0.4853986	4.3150087	-2.3551131	F	0.518965	4.315900	-2.316179
F	-0.8114901	-4.7201011	-0.6844768	F	-0.681481	-4.802325	-0.781857
F	-1.8208639	-3.0315423	-1.6386552	F	-1.829057	-3.100213	-1.486730
F	-0.2686080	-4.1222214	-2.7168912	F	-0.327561	-3.997033	-2.768276
F	3.7067943	-1.8160581	1.1197627	F	3.756911	-1.814241	0.948597
F	4.2904660	-0.1236783	2.3710996	F	4.253507	-0.204988	2.315021
F	5.5375319	-0.7085335	0.6728427	F	5.534826	-0.615562	0.609973
F	-5.4601837	0.2694969	1.4082325	F	-5.452884	0.348696	1.314028
F	-4.7025644	0.7248250	-0.5911337	F	-4.673138	0.708749	-0.679923
F	-3.8495874	1.7247838	1.1576922	F	-3.826109	1.755669	1.024406

Sn(OTf)4(CH3NO2)

TPSS				B3LYP			
40				40			
Energy = -4306.753701794				Energy = -4305.26701325			
Sn	-0.0043768	0.0117789	-0.0375016	Sn	0.012188	0.043407	-0.061945
O	1.8201039	-0.0335699	0.8366514	O	1.862078	0.150544	0.719888
S	3.2883854	0.3138365	0.3793879	S	3.310237	0.444561	0.216323
O	3.7780894	1.4166236	1.1629682	O	3.819064	1.599770	0.881745
O	3.4153528	0.2778968	-1.0545395	O	3.402193	0.290477	-1.200988
C	4.1487667	-1.2144425	1.0681062	C	4.177992	-1.014392	1.005490
O	-2.0079068	0.0990079	-0.4495754	O	-1.991720	-0.015827	-0.402366
S	-3.3311862	-0.3758258	0.2333293	S	-3.276349	-0.538955	0.284270
O	-4.2099930	-0.9179964	-0.7651382	O	-4.136477	-1.123081	-0.689742
O	-3.0897331	-1.0834122	1.4721587	O	-2.985184	-1.228178	1.510586
C	-4.0652640	1.2884229	0.7173174	C	-4.072384	1.080840	0.775292
O	-0.1768975	2.2130525	0.4516093	O	-0.302719	2.226049	0.461354
S	-0.1852329	2.6559731	-0.9941342	S	-0.327635	2.699017	-0.959292
O	-1.3347161	3.3485762	-1.4932155	O	-1.497141	3.346383	-1.439711
O	0.2403147	1.3804179	-1.7138013	O	0.140715	1.463679	-1.695588
C	1.2671014	3.8493092	-1.1902835	C	1.069316	3.939829	-1.132244

O	0.5492596	-1.3274683	-1.6792196	O	0.533499	-1.248802	-1.735596
S	0.2905269	-2.6425458	-0.9620739	S	0.445419	-2.579587	-1.031583
O	1.3467118	-3.6060065	-0.9084959	O	1.576559	-3.435384	-1.072675
O	-0.3142782	-2.1704377	0.3459478	O	-0.089622	-2.170087	0.310927
C	-1.1133681	-3.4579090	-1.9305812	C	-0.941617	-3.503462	-1.895357
O	-0.6362775	0.1775298	2.1220829	O	-0.553919	0.114431	2.105235
N	-0.4502046	-0.6444573	3.0737351	N	-0.313243	-0.694984	3.037519
O	0.3347085	-1.5554526	3.0656335	O	0.542037	-1.523259	3.021198
C	-1.3463257	-0.4006763	4.2506558	C	-1.225857	-0.554451	4.205828
H	-0.9760854	-1.0142862	5.0679798	H	-0.833191	-1.175927	5.002393
H	-1.3204272	0.6674267	4.4638346	H	-1.264219	0.500107	4.466025
H	-2.3436569	-0.6984745	3.9177835	H	-2.201724	-0.888620	3.853935
F	-5.2428975	1.0605375	1.3241435	F	-5.229878	0.808162	1.377693
F	-3.2542227	1.9309333	1.5794372	F	-3.286652	1.741727	1.630784
F	-4.2626723	2.0561684	-0.3564692	F	-4.295240	1.836790	-0.289815
F	-2.0944016	-2.5876706	-2.1596855	F	-2.019683	-2.743603	-1.983522
F	-1.5759432	-4.4905451	-1.2164706	F	-1.213682	-4.597516	-1.193430
F	-0.6170892	-3.8986230	-3.0910633	F	-0.523879	-3.839201	-3.108709
F	3.9496685	-1.3060075	2.3933922	F	4.043872	-0.966995	2.331102
F	5.4631972	-1.0885041	0.8304637	F	5.469663	-0.943337	0.693615
F	3.6981567	-2.3272034	0.4781615	F	3.677990	-2.160414	0.556736
F	2.3911225	3.3143387	-0.7232347	F	2.209715	3.416006	-0.720673
F	1.4011394	4.1369661	-2.4887267	F	1.162041	4.288805	-2.408467
F	0.9776546	4.9649881	-0.5090459	F	0.767527	5.003408	-0.395475

Sn(OTf)4(HCOOCH3)

TPSS				B3LYP			
41				41			
Energy = -4290.807581835				Energy = -4289.33331727			
Sn	0.0320756	0.3146545	-0.7134804	Sn	0.081070	0.022173	-0.204844
O	1.8260106	-0.6463332	-0.5680324	O	-1.915979	0.294379	0.018441
S	2.5421735	-1.2455792	0.6876059	S	-2.826760	0.359040	1.269868
O	1.6687616	-2.1343225	1.4236668	O	-2.322959	1.298079	2.232079
O	3.3084768	-0.2456842	1.3885451	O	-3.227458	-0.946549	1.693982
O	-1.7265891	1.3288304	-0.9278325	O	2.067803	-0.278696	-0.476882
S	-3.0317364	1.4253962	-0.0732261	S	3.344369	-0.121852	0.385585
O	-4.1664126	1.4925436	-0.9501915	O	4.403753	0.394831	-0.413825
O	-3.0064713	0.5146923	1.0515561	O	3.041304	0.449385	1.668375
O	1.0079972	2.2360571	-0.1080792	O	-0.177240	-2.192709	0.028293
S	1.2225051	2.7435987	-1.5167904	S	-0.248189	-2.499647	-1.436750
O	0.6949542	4.0282310	-1.8648691	O	0.659413	-3.452119	-1.971929
O	0.7970392	1.5483055	-2.3537378	O	-0.254787	-1.117216	-2.037461
O	-0.3233298	-0.8956419	-2.5200005	O	0.011217	1.574482	-1.748129
S	-0.9071621	-2.1154087	-1.8347835	S	0.164082	2.786116	-0.868789
O	-0.2669182	-3.3787113	-2.0406492	O	-0.850987	3.777604	-0.920059

O	-1.0814327	-1.6248042	-0.4115066	O	0.482542	2.162084	0.457100
O	-0.0671060	0.3387934	1.4387783	O	0.200633	-0.307051	1.906018
C	-0.6244088	-0.4771463	2.2082420	C	0.467813	0.481368	2.829749
H	-1.2289338	-1.3172624	1.8720005	H	0.782851	1.508548	2.670702
O	-0.5192584	-0.3808563	3.4940544	O	0.388174	0.140188	4.064467
C	0.3169657	0.7091825	4.0293333	C	-0.068191	-1.208740	4.391042
H	0.2711372	0.5723933	5.1067322	H	-0.072524	-1.240750	5.474722
H	1.3310945	0.5931006	3.6457257	H	-1.065913	-1.356656	3.984054
H	-0.1112669	1.6639106	3.7230800	H	0.627885	-1.933748	3.975946
C	-2.8252262	3.1514858	0.6469364	C	3.750513	-1.919440	0.702183
C	3.0943092	2.8551798	-1.7427389	C	-1.971925	-3.176217	-1.739331
C	3.7647548	-2.3303257	-0.2493818	C	-4.310724	1.155645	0.453075
C	-2.6561453	-2.2803525	-2.5262321	C	1.749744	3.610665	-1.437331
F	-3.9054165	3.4302694	1.3926764	F	4.866972	-1.976008	1.425158
F	-2.7085348	4.0628250	-0.3231303	F	3.928669	-2.568757	-0.440591
F	-1.7312759	3.2019180	1.4332831	F	2.759425	-2.498227	1.387905
F	-2.5694786	-2.6363151	-3.8120418	F	1.564871	4.073482	-2.666971
F	-3.2958339	-3.2326403	-1.8369233	F	2.015814	4.617228	-0.612409
F	-3.3132371	-1.1259737	-2.4192822	F	2.749327	2.743758	-1.426683
F	3.1189774	-3.2267679	-1.0031359	F	-3.983822	2.341334	-0.047110
F	4.5189278	-2.9724566	0.6564351	F	-5.252575	1.310550	1.381730
F	4.5554755	-1.5797728	-1.0285295	F	-4.775205	0.376221	-0.519424
F	3.6752280	1.6893477	-1.4607209	F	-2.888071	-2.322534	-1.311761
F	3.3470964	3.1908338	-3.0131282	F	-2.119499	-3.379729	-3.043204
F	3.5634989	3.8049137	-0.9249097	F	-2.089088	-4.328179	-1.089075

Sn(OTf)4((MeOOC)2CMe2)
TPSS
56
Energy = -4636.822236242

Sn	-0.0027202	-0.0011059	-0.0822362
O	-1.9108946	0.7606487	-0.1016131
S	-2.8208261	1.3302157	1.0120837
O	-3.0818059	0.3356666	2.0372399
O	-2.4264043	2.6593318	1.4150690
C	-4.3995727	1.4974040	0.0004257
O	-0.5046174	-1.4256370	-1.4201151
O	1.9027901	-0.7693613	-0.1243102
O	0.4863243	1.4357515	-1.4114930
S	-1.8574718	-2.1465468	-1.7317628
S	2.8242859	-1.3368362	0.9808323
S	1.8423588	2.1377458	-1.7514632
O	-2.5338553	-2.5516044	-0.5202596
O	3.0961198	-0.3404789	2.0014448
O	2.5483785	2.5350319	-0.5542789

O	-2.5712450	-1.4873569	-2.7914903
O	2.4333969	-2.6649405	1.3904797
O	2.5261220	1.4685922	-2.8246203
C	-1.0985741	-3.7052510	-2.4644701
C	4.3925905	-1.5073621	-0.0464447
C	1.0887617	3.7056630	-2.4699661
O	0.5168655	1.2773646	1.5595079
C	0.6604438	1.0875360	2.7895068
C	0.0188514	-0.0035915	3.6431381
O	1.3494611	1.9359411	3.4964064
C	-1.0396294	0.6853052	4.5602984
C	1.0854726	-0.6924130	4.5505549
C	-0.6314302	-1.0942200	2.7952496
C	2.0013640	3.0498866	2.7765945
O	-1.3097031	-1.9452875	3.5094585
O	-0.5045324	-1.2810107	1.5630707
H	2.5729636	3.5582050	3.5492803
H	2.6338844	2.6388170	1.9912093
H	1.2260465	3.6905325	2.3555150
C	-1.9705669	-3.0581106	2.7960325
H	-2.5211856	-3.5759429	3.5775839
H	-2.6233468	-2.6446904	2.0287598
H	-1.2014579	-3.6903797	2.3517834
H	-1.5158942	-0.0795333	5.1758378
H	-0.5214967	1.3955901	5.2075810
H	-1.8048553	1.2011448	3.9794084
H	0.5732805	-1.4026011	5.2026334
H	1.8451810	-1.2084638	3.9626509
H	1.5675362	0.0723514	5.1616234
F	-4.8062588	0.3034854	-0.4399694
F	-5.3433090	2.0181657	0.8043097
F	-4.2035662	2.3178946	-1.0376272
F	0.3573546	4.3446843	-1.5409122
F	0.3130971	3.4267848	-3.5244899
F	2.0921046	4.5094318	-2.8611835
F	4.1879508	-2.3380237	-1.0747707
F	4.7906517	-0.3163953	-0.5020977
F	5.3465954	-2.0178545	0.7519520
F	-2.0989891	-4.5273921	-2.8240056
F	-0.3577911	-3.4180740	-3.5416507
F	-0.3307781	-4.3278479	-1.5539860

Sn(OTf)4[1] (eta 1)
TPSS
76

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Energy = -4949.014638644
Sn   -0.0407658   -0.3180930    0.6576601
O     1.9324194   -0.8405217    0.7230198
S     3.2563442   -0.0170671    0.7991788
O     4.2087115   -0.5560869   -0.1352382
O     2.9932665    1.4033020    0.8600606
C     3.8566247   -0.5472650    2.5019572
O    -2.0333293    0.0624969    0.5021986
S    -2.9554304    0.4465621   -0.7004709
O    -2.6379156    1.7707617   -1.1888496
O    -3.1183643   -0.6490646   -1.6216840
C    -4.5609280    0.6090943    0.2753265
O     2.8819415    1.6057288   -4.8477265
C     2.4002670    1.5035111   -3.7428759
C     0.9047938    1.1826931   -3.4966616
O     3.0831137    1.6103383   -2.5899935
C     0.6856034   -0.3233183   -3.8655316
C     0.0687209    2.0998493   -4.4637160
C     0.5729343    1.4848462   -2.0434064
C     4.5184471    1.8297243   -2.7223323
O     0.5423089    2.7492475   -1.7523067
O     0.3366405    0.5555511   -1.2178364
H     4.8814788    1.9177731   -1.7008830
H     4.9687689    0.9735954   -3.2270812
H     4.6962770    2.7419415   -3.2949823
C     0.2813649    3.2063737   -0.3800949
H     0.3602150    4.2891922   -0.4453552
H    -0.7271100    2.9096196   -0.0951778
H     1.0465287    2.7961416    0.2791798
H     0.6291036   -0.3495120   -4.9558321
C     1.7355395   -1.2771546   -3.3652994
H    -0.3055966   -0.6063085   -3.4921980
C    -1.3918302    1.7620010   -4.5316175
H     0.2013396    3.1391129   -4.1401173
H     0.5594054    1.9999742   -5.4338477
H     1.7985928   -1.3935195   -2.2854633
H    -1.9549267    1.9119752   -3.6107448
C    -2.0735177    1.3310249   -5.6070198
C     2.5794003   -2.0124566   -4.1099254
C     3.5570227   -2.9497888   -3.4442500
H     3.3769990   -3.9861696   -3.7607995
H     4.5877639   -2.7082064   -3.7366039
H     3.4877427   -2.9016896   -2.3546127
C     2.6450172   -2.0059435   -5.6153914
H     2.4405033   -3.0113829   -6.0072305
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H     1.9463858   -1.3083432   -6.0808041
H     3.6560984   -1.7389122   -5.9486229
C    -3.5563059    1.0694245   -5.5120753
H    -3.9369460    1.2614772   -4.5057704
H    -4.1086781    1.7003759   -6.2215479
H    -3.7839276    0.0277051   -5.7748641
C    -1.4784789    1.0784935   -6.9687302
H    -1.9716363    1.7083652   -7.7210337
H    -0.4047021    1.2714708   -7.0198983
H    -1.6536583    0.0378126   -7.2725539
O    -0.4111043   -2.0195309    1.9724666
O     0.1709331    1.0422873    2.1359824
S    -0.3565747   -3.0734880    0.8759729
C    -2.0712701   -3.8705131    0.8642780
O    -0.2958439   -2.2179455   -0.3829680
O     0.5882315   -4.1392628    1.0084432
S    -0.9253120    1.7017806    3.0614533
C     0.2402714    2.2092206    4.4533088
O    -1.4086195    2.9231467    2.4668525
O    -1.8259348    0.7176847    3.6019794
F     2.9534167   -0.2358959    3.4427083
F     5.0046210    0.0979715    2.7635292
F     4.0779822   -1.8680849    2.5248852
F     1.2159492    3.0045572    3.9914488
F     0.7823143    1.1316221    5.0334977
F    -0.4824509    2.8824612    5.3619929
F    -3.0216229   -2.9414789    0.8060949
F    -2.1519503   -4.6759938   -0.1993931
F    -2.2023198   -4.5871689    1.9852056
F    -5.5273974    0.9348807   -0.5997603
F    -4.4591154    1.5683111    1.1986022
F    -4.8757529   -0.5508844    0.8652470

Sn(OTf)4[1] (eta 2)
TPSS
76
Energy = -4949.031081843
Sn   -0.4208152    0.3415647   -2.4783616
O    -0.4286244    2.3914457   -2.3401093
S     0.0286706    3.3659146   -1.2313396
O    -0.7147337    3.1523793   -0.0034123
O     1.4661790    3.4861057   -1.1652537
C    -0.6261476    4.9556713   -1.9957637
O    -2.2099081    0.3501590   -3.4201363
O    -0.4019047   -1.6961462   -2.7551611
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O	0.7023271	0.5912756	-4.1403929
S	-3.5169448	1.1878314	-3.2654368
S	-0.3715649	-2.8962068	-1.7838111
S	1.6910577	-0.3552361	-4.8942202
O	-3.6277780	1.7764376	-1.9499222
O	0.8082939	-2.8548790	-0.9367875
O	2.6637526	-0.9310751	-3.9929547
O	-3.7601587	1.9646728	-4.4495437
O	-1.6570857	-3.1501372	-1.1799437
O	1.0124464	-1.1706888	-5.8652625
C	-4.7342517	-0.2455589	-3.2992842
C	-0.0807020	-4.2537768	-3.0540223
C	2.5868195	0.9983379	-5.8461550
O	1.3356141	0.2193508	-1.2629873
C	1.5323214	-0.1201740	-0.0697554
C	0.5734870	0.0410261	1.1027745
O	2.7013345	-0.5818858	0.2728621
C	1.0718281	1.2758218	1.9818662
C	0.5809125	-1.3049008	1.9580349
C	-0.8455075	0.3011182	0.6171616
C	3.7045729	-0.7545300	-0.7974322
O	-1.6582224	0.6411030	1.5714706
O	-1.2988877	0.1203795	-0.5451166
H	4.5551684	-1.1982177	-0.2854889
H	3.2920933	-1.4092337	-1.5631747
H	3.9438889	0.2239280	-1.2142578
C	-3.0717698	0.8772961	1.2229862
H	-3.5209977	1.1885626	2.1630779
H	-3.1194341	1.6531139	0.4606994
H	-3.5022921	-0.0546538	0.8559127
H	0.2185537	1.5695095	2.5923891
C	2.2808562	1.0161571	2.8318327
H	1.2618543	2.1060792	1.2927578
C	-0.2879872	-1.3105088	3.1762033
H	0.3576170	-2.1342813	1.2861297
H	1.6283016	-1.4035248	2.2647035
H	3.1742063	0.6821589	2.3077420
H	-0.0626939	-0.5453729	3.9174503
C	-1.2453321	-2.2062349	3.4772601
C	2.3926331	1.2344573	4.1542224
C	3.7081831	0.9962720	4.8532894
H	4.0745699	1.9208789	5.3185392
H	3.5901241	0.2632177	5.6623614
H	4.4736975	0.6307421	4.1633686
C	1.2953073	1.7476971	5.0503104

H	1.5796460	2.7209597	5.4715994
H	0.3360990	1.8733110	4.5431803
H	1.1499084	1.0705647	5.9019939
C	-1.9643150	-2.1277243	4.8015047
H	-1.6147269	-1.2866079	5.4068793
H	-3.0470719	-2.0230251	4.6501441
H	-1.8193995	-3.0520033	5.3764368
C	-1.6818808	-3.3458840	2.5944853
H	-2.7696391	-3.3159670	2.4494064
H	-1.2136022	-3.3508573	1.6094420
H	-1.4624103	-4.3054196	3.0815616
F	-1.0717052	-4.2727443	-3.9516120
F	-0.0571362	-5.4275664	-2.3966561
F	1.0883465	-4.0769009	-3.6772886
F	3.5409691	0.4192671	-6.5954882
F	1.7431170	1.6610275	-6.6473428
F	3.1666664	1.8674396	-5.0012814
F	-0.3203083	5.9655079	-1.1619986
F	-1.9528602	4.8970891	-2.1474748
F	-0.0481365	5.1756980	-3.1827841
F	-4.5076368	-1.0755449	-2.2641028
F	-4.6381233	-0.9355435	-4.4419245
F	-5.9787281	0.2514820	-3.1885986

Sn(OTf)4(DMSO)

TPSS

43

Energy = -4614.966221999

Sn	0.0867259	0.5880877	-0.6545448
O	2.0251547	-0.0980846	-0.5410740
S	3.1446328	0.0000906	0.5358363
O	2.5876605	-0.0194657	1.8759052
O	4.1405418	0.9762596	0.1903787
C	3.9306278	-1.6883983	0.2587071
O	-1.7806404	1.4166233	-0.8095641
S	-3.2193248	0.8717175	-0.5697871
O	-4.0378590	1.1181402	-1.7244093
O	-3.2047954	-0.4231259	0.0736444
C	-3.7747694	2.1012626	0.7400655
O	0.7689405	2.5778132	-0.0386259
S	0.7440741	3.1770368	-1.4420247
O	-0.1030765	4.3087753	-1.6607644
O	0.5477664	1.9418845	-2.3067811
C	2.5130876	3.7539730	-1.8116509
O	-0.3204948	-0.8633179	-2.0231213

B3LYP

43

Energy = -4613.46163385

Sn	-0.035405	0.362272	-0.144109
O	1.904503	-0.285422	-0.015356
S	3.036981	-0.225940	1.028426
O	2.510603	-0.327623	2.364974
O	3.994277	0.785344	0.721861
C	3.849049	-1.869158	0.654083
O	-1.910624	1.146633	-0.312811
S	-3.337739	0.611231	-0.084629
O	-4.145814	0.839474	-1.236349
O	-3.320340	-0.671467	0.559967
C	-3.911882	1.832627	1.208342
O	0.612613	2.367636	0.437061
S	0.612195	2.945869	-0.961064
O	-0.229719	4.061239	-1.207563
O	0.427567	1.704864	-1.797340
C	2.372604	3.518629	-1.306782
O	-0.436419	-1.127991	-1.450546

S	-0.0533210	-2.3928635	-1.8594927	S	-0.194549	-2.650883	-1.331266
O	1.1046265	-2.8173639	-2.5951506	O	0.968445	-3.061571	-2.045299
O	-0.2297722	-2.7807691	-0.4704757	O	-0.399366	-3.074946	0.030505
C	-1.5542277	-3.0310549	-2.8024310	C	-1.672216	-3.246231	-2.313805
O	-0.4402417	0.0264719	1.2545665	O	-0.540775	-0.212821	1.750369
S	-0.0277018	-1.2495049	2.0979169	S	-0.185058	-1.482189	2.609189
C	-1.6071456	-2.0863557	2.3265326	C	-1.782288	-2.268228	2.824725
H	-1.8841188	-2.4967729	1.3561071	H	-2.066844	-2.669014	1.855711
H	-1.4295073	-2.8907962	3.0471495	H	-1.637878	-3.078166	3.541781
H	-2.3526672	-1.3751160	2.6842611	H	-2.512444	-1.542287	3.175181
C	0.1600620	-0.5099694	3.7300879	C	0.029351	-0.739532	4.227762
H	1.0602020	0.1028483	3.6895163	H	0.950834	-0.164768	4.186618
H	-0.7286037	0.0818467	3.9580283	H	-0.829919	-0.110619	4.454558
H	0.2874352	-1.3308016	4.4419072	H	0.124828	-1.553522	4.947539
F	-1.5265872	-2.5970755	-4.0676723	F	-1.604380	-2.796133	-3.561269
F	-1.5015267	-4.3735684	-2.7925950	F	-1.644651	-4.578739	-2.321575
F	-2.6891040	-2.6317772	-2.2170559	F	-2.802518	-2.833745	-1.751832
F	-5.0359056	1.8072943	1.0984535	F	-5.160971	1.527269	1.558746
F	-2.9873958	2.0143245	1.8335860	F	-3.131929	1.758864	2.295502
F	-3.7302359	3.3547764	0.2749093	F	-3.877701	3.073517	0.737684
F	2.9345589	4.5131051	-0.7952471	F	2.754035	4.318238	-0.319098
F	2.4734104	4.4826859	-2.9323419	F	2.358330	4.191484	-2.450548
F	3.3226060	2.7147620	-1.9784547	F	3.186002	2.486076	-1.402600
F	4.3762098	-1.8022803	-0.9951201	F	4.281140	-1.899331	-0.599039
F	4.9640942	-1.8052541	1.1100302	F	4.882677	-2.014339	1.483512
F	3.0466055	-2.6660634	0.5107946	F	2.987203	-2.864278	0.854050

Sn(OTCl)4(DMSO)2 TPSS
41
Energy = -5658.089845733

Sn	0.0359461	0.1715998	-0.0721595
O	0.5973445	-1.5567135	-1.1181811
S	-0.0110389	-2.9632668	-1.2348545
O	-0.6949671	-3.3504662	-0.0203920
O	-0.6453344	-3.1447271	-2.5147841
Cl	1.7372259	-4.0848764	-1.2994545
O	2.0602669	0.5344082	0.1252098
O	-0.4513118	1.9828224	0.7796193
O	-1.9296186	-0.2783104	-0.5350374
S	3.2000324	-0.1694655	0.8982699
S	-0.0139610	3.4369661	0.4782746
S	-3.2652594	0.1109337	0.1399404
O	2.8569417	-1.5143550	1.2873065
O	-0.1016971	4.2041538	1.6886981
O	-3.0961525	0.2978853	1.5658599

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O     4.4424687    0.1140415    0.2335593
O     1.1665203    3.4958689   -0.3503777
O    -3.9815197    1.0810308   -0.6378547
Cl    3.2201257    0.9487588    2.6629880
Cl   -1.5877485    4.0781513   -0.7307649
Cl   -4.2759465   -1.6891177   -0.0908855
O    -0.0026710   -0.6310899    1.8306457
S    -1.0086226   -1.6475888    2.4909785
C    -1.3996127   -0.7942031    4.0289847
H    -2.0088620    0.0664645    3.7515722
H    -1.9773950   -1.4858873    4.6488493
H    -0.4711392   -0.4937693    4.5184851
C     0.1168620   -2.9116099    3.1113403
H     0.4749737   -3.4579072    2.2385707
H     0.9380890   -2.4320444    3.6466768
H    -0.4654925   -3.5712937    3.7614091
O     0.1350704    1.0588646   -1.9638249
S     1.3462645    0.8088410   -2.9330726
C     0.5410308    0.0854720   -4.3752618
H     0.2083245   -0.9115935   -4.0777811
H     1.2871410    0.0151700   -5.1720807
H    -0.3033890    0.7128171   -4.6683459
C     1.6812195    2.4749434   -3.5289585
H     2.0364729    3.0377861   -2.6635938
H     0.7615253    2.9096389   -3.9255783
H     2.4596506    2.4013678   -4.2937034

Sn(OTCl)4(DMSO)3 TPSS
51
Energy = -6211.434894543
Sn    0.1097467    0.0941269   -0.0261390
O    -2.0050642   -0.6756927   -0.1420342
S    -3.2190177   -0.7848541   -1.0432127
O    -4.3089609    0.0370051   -0.5747744
O    -2.8887590   -0.7974919   -2.4510913
Cl   -3.8151453   -2.7635849   -0.5958848
O     0.3729767   -1.8751114    0.7095660
O     1.7519172    0.9949924   -1.1251250
O    -0.8134150    1.7719793   -0.9247143
S     0.4960861   -2.5765165    2.0664641
S     3.1072043    0.3911460   -1.4756198
S    -0.3537973    3.2278314   -0.7824551
O     0.2279722   -1.7077697    3.1897159
O     4.1708324    1.3167093   -1.1680100
O     0.3895105    3.4273976    0.4496976
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O    -0.1286824   -3.8710951    1.9914156
O     3.2265978   -0.9942658   -1.0776757
O     0.1219578    3.7859922   -2.0146290
Cl    2.5571994   -2.9633425    2.1334425
Cl    3.0089727    0.3630225   -3.5791272
Cl   -2.2200568    4.1382915   -0.4402034
O    -0.8567719    0.7520736    1.7754384
S    -2.3622835    1.1951645    1.8217540
C    -2.2821018    2.5020235    3.0647171
H    -1.7033694    3.3130764    2.6198859
H    -3.3056805    2.8338950    3.2590460
H    -1.8066902    2.1220794    3.9711840
C    -3.1598310   -0.0941464    2.8031462
H    -3.2179603   -0.9787774    2.1691958
H    -2.5632988   -0.2853624    3.6972660
H    -4.1652514    0.2594145    3.0479408
O     0.2458528   -0.9525220   -1.8541874
S    -0.2797061   -2.4058700   -2.1377552
C    -0.5324979   -2.3133517   -3.9203065
H    -1.3897704   -1.6576864   -4.0709060
H    -0.7538809   -3.3248585   -4.2720644
H     0.3727507   -1.9137256   -4.3816331
C     1.2168219   -3.4177395   -2.1099350
H     1.5434578   -3.4731927   -1.0717766
H     1.9822702   -2.9522476   -2.7325027
H     0.9357350   -4.4100353   -2.4753803
O     1.7078558    0.4354822    1.4049699
S     1.8735380    1.5377740    2.4906684
C     3.2270422    2.5637965    1.8770512
H     2.8291022    3.1242294    1.0303381
H     3.5115232    3.2440230    2.6856437
H     4.0576918    1.9266926    1.5685694
C     2.7486237    0.6279693    3.7819096
H     2.0483351   -0.1188167    4.1598413
H     3.6289954    0.1489419    3.3490111
H     3.0222630    1.3399348    4.5658298

Sn(OTCl)4(DMSO)4 TPSS (1)
61
Energy = -6764.804075735
Sn    0.0000000    0.0000000    0.0000000
O    -0.7293529    1.0837537   -1.6130684
O    -0.1534743    1.6179978    1.2464705
S    -0.9613338    2.6380754   -1.7657889
S    -0.4839411    1.4124799    2.8252653
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C	-2.2807420	2.6611168	-2.9894716
C	-1.6974348	2.7297017	3.0339901
H	-3.1635223	2.2515070	-2.4955055
H	-2.5857141	2.4187992	2.4810153
H	-2.4456427	3.7090211	-3.2577423
H	-1.9041833	2.8010860	4.1023530
H	-1.9640991	2.0663935	-3.8507176
H	-1.2838075	3.6540370	2.6259615
C	0.4290033	3.1729495	-2.7811120
C	0.9890828	2.1872011	3.5223920
H	1.3244522	3.0690653	-2.1650285
H	1.8170875	1.5035188	3.3312083
H	0.4685041	2.5487181	-3.6791992
H	1.1418519	3.1368860	3.0057266
H	0.2567449	4.2270164	-3.0205948
H	0.8287482	2.3090490	4.5939628
O	0.7293529	-1.0837537	1.6130684
O	0.1534743	-1.6179978	-1.2464705
S	0.9613338	-2.6380754	1.7657889
S	0.4839411	-1.4124799	-2.8252653
C	2.2807420	-2.6611168	2.9894716
C	1.6974348	-2.7297017	-3.0339901
H	3.1635223	-2.2515070	2.4955055
H	2.5857141	-2.4187992	-2.4810153
H	2.4456427	-3.7090211	3.2577423
H	1.9041833	-2.8010860	-4.1023530
H	1.9640991	-2.0663935	3.8507176
H	1.2838075	-3.6540370	-2.6259615
C	-0.4290033	-3.1729495	2.7811120
C	-0.9890828	-2.1872011	-3.5223920
H	-1.3244522	-3.0690653	2.1650285
H	-1.8170875	-1.5035188	-3.3312083
H	-0.4685041	-2.5487181	3.6791992
H	-1.1418519	-3.1368860	-3.0057266
H	-0.2567449	-4.2270164	3.0205948
H	-0.8287482	-2.3090490	-4.5939628
O	1.9077907	0.6966022	-0.5560919
O	-1.9077907	-0.6966022	0.5560919
S	3.2587186	0.2231160	0.0116258
S	-3.2587186	-0.2231160	-0.0116258
O	3.5603849	0.8425085	1.2778523
O	-3.5603849	-0.8425085	-1.2778523
O	3.4213360	-1.2090844	-0.1312478
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Cl	4.5035947	1.0983445	-1.3951322

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Cl   -4.5035947   -1.0983445    1.3951322
O     1.1075673   -0.9672775   -5.3152773
S     0.4253337    0.1817293   -5.9450077
O    -0.3146383    1.0070835   -4.9823093
O     1.1810231    0.8808961   -6.9581278
Cl   -1.1652262   -0.7890985   -7.0320250
O    -1.1075673    0.9672775    5.3152773
S    -0.4253337   -0.1817293    5.9450077
O     0.3146383   -1.0070835    4.9823093
O    -1.1810231   -0.8808961    6.9581278
Cl    1.1652262    0.7890985    7.0320250

Sn(OTCl)4(DMSO)4 TPSS (2)
61
Energy = -6764.791740516
Sn   -0.3668732   -0.0237414    0.0271125
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S     0.6688673    2.7387870    1.5802425
C     2.4133542    3.0283206    1.2386827
H     2.5711069    2.8579950    0.1749080
H     2.5923724    4.0788435    1.4909164
H     3.0186570    2.3461075    1.8408349
C     0.6987195    2.9548116    3.3712956
H    -0.3079515    2.7435728    3.7333543
H     1.4346020    2.2674547    3.7933116
H     0.9680604    3.9970981    3.5641595
O     0.8814539   -0.9528978   -1.3654503
S     2.0222745   -0.4239739   -2.3234544
C     3.2150305   -1.7692675   -2.2260225
H     3.5838871   -1.7997284   -1.1980946
H     4.0290619   -1.5105851   -2.9098436
H     2.7240404   -2.6993407   -2.5191757
C     1.3246336   -0.7895010   -3.9508296
H     0.5255376   -0.0672539   -4.1203398
H     0.9526886   -1.8153236   -3.9633762
H     2.1277758   -0.6411049   -4.6793141
O     0.5051773   -1.3228160    1.4435893
S     0.5961641   -2.8867780    1.3844068
C    -0.8499351   -3.4624759    2.3051182
H    -0.7110794   -4.5328888    2.4831062
H    -1.7209070   -3.2930870    1.6720371
H    -0.9219418   -2.8998747    3.2379454
C     1.8689621   -3.1790451    2.6237102
H     1.5809231   -2.6789842    3.5506798
H     2.7992840   -2.7699517    2.2165527
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H     1.9426450   -4.2626806    2.7559171
O    -1.8827835    0.8988600   -1.0997143
S    -3.4125202    0.5265230   -1.1007516
C    -4.1823356    1.9413607   -0.2848599
H    -5.2648719    1.8183943   -0.3821692
H    -3.8917810    1.9072914    0.7658309
H    -3.8324054    2.8579614   -0.7631223
C    -3.8344644    0.9098711   -2.8118939
H    -3.4358124    1.8960073   -3.0578274
H    -3.3780741    0.1287665   -3.4200120
H    -4.9246217    0.8775458   -2.8936833
O    -2.0716626   -0.1059251    1.4182028
S    -2.3249748    0.3745353    2.8340205
O    -2.4191715    1.8202174    2.9109771
O    -1.5670596   -0.3322652    3.8370159
Cl   -4.3091938   -0.3077946    3.0372799
O     3.5434282    0.3981957   -0.0200896
S     4.2449570   -0.2939202    1.0683284
O     4.1848358   -1.7570699    0.9732018
O     4.0398619    0.2681866    2.3962757
Cl    6.3053443    0.1283676    0.6455173
O     0.4958686    1.8464173   -1.0154835
S     0.3533457    2.7405864   -2.2278724
O     1.5192422    3.5758042   -2.3813172
O    -0.1953497    2.0629302   -3.3835414
Cl   -1.1702126    4.1040827   -1.6288518
O    -1.4224349   -1.9147158   -0.4493271
S    -1.9807189   -2.6254583   -1.6674341
O    -3.1203637   -3.4300872   -1.3065885
O    -2.0485950   -1.7689743   -2.8344785
Cl   -0.4679651   -4.0305009   -2.1145424

Sn(OTCl)4(DMSO)5 TPSS
71
Energy = -7318.155194057
Sn    0.7655168   -0.0160985    0.1175825
O    -0.7613668   -0.7345670    1.2945093
S    -0.6993613   -1.7146249    2.5500014
C    -1.4569271   -3.2133611    1.8890588
H    -0.7202490   -3.6882244    1.2388400
H    -1.6695194   -3.8604103    2.7453309
H    -2.3677749   -2.9374180    1.3479342
C    -2.0592084   -1.1018331    3.5463081
H    -1.7665154   -0.1055408    3.8858729
H    -2.9698650   -1.0838689    2.9412614
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O	-0.2770349	1.7758249	-0.0676866
S	3.2810599	1.0948013	1.9427153
S	-1.8781090	1.6285822	-0.1692867
C	3.7348677	0.3367414	3.5103693
C	-2.2681741	2.6760868	-1.5773665
H	3.8239947	-0.7327412	3.3145195
H	-1.8403770	2.2125715	-2.4706318
H	4.7075623	0.7522058	3.7904942
H	-3.3593288	2.6826558	-1.6432791
H	2.9625770	0.5638382	4.2494213
H	-1.8641938	3.6766357	-1.4085098
C	3.1254779	2.8191393	2.4429988
C	-2.4555817	2.6472445	1.1955835
H	2.7507556	3.3629525	1.5732946
H	-2.0142616	2.2402159	2.1088099
H	2.4466895	2.8839748	3.3018296
H	-2.1511920	3.6836518	1.0367153
H	4.1335009	3.1646942	2.6931344
H	-3.5424405	2.5293761	1.2161563
O	2.3010928	0.7778035	-1.0309334
S	1.9862879	1.2875531	-2.5303861
C	2.6250689	2.9729267	-2.4411657
H	1.9356642	3.5323531	-1.8066774
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C	3.3202078	0.4824913	-3.4369977
H	3.0973926	-0.5845182	-3.4354134
H	4.2622477	0.6884788	-2.9249911
H	3.2880864	0.8796101	-4.4522083
O	-0.2173669	-0.6052152	-1.6320629
S	-0.9797654	-1.9617225	-1.9514941
C	-2.3635995	-1.3751660	-2.9358294
H	-3.0538593	-0.8791919	-2.2503045
H	-2.8396388	-2.2670720	-3.3543072
H	-1.9805524	-0.7073867	-3.7123915
C	0.0361786	-2.6974210	-3.2460882
H	0.9791984	-2.9971310	-2.7841654
H	0.1830515	-1.9633685	-4.0443594
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S	3.0263467	-2.4390951	-0.0844914
O	3.2202679	-2.6180637	-1.5038787
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O	1.6014881	-1.9515008	0.2327481

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Cl    2.8768679   -4.3456413    0.7295955
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O    -3.7573852   -1.7981572   -0.0427776
O    -4.4446161    0.4271624   -0.8518572
Cl   -6.5522764   -1.2512356    0.0842879
S     0.1581197    1.1715706   -5.2468670
O    -1.1171528    1.3813181   -4.5674622
O     1.2036443    2.1621961   -4.9177877
O     0.6440629   -0.2101146   -5.2466669
Cl   -0.2560490    1.5808443   -7.2777120
S     0.2673013    1.4902196    4.9761038
O     0.5981123    0.0636018    4.9176571
O    -0.8252964    1.8998958    4.0907738
O     1.4295503    2.3818539    4.9879511
Cl   -0.5610957    1.7341335    6.9257169

Sn(OTCl)4(DMSO)6 TPSS
81
Energy = -7871.505574357
Sn    0.0000000    0.0000000    0.0000000
O    -2.0468349   -0.1895874    0.1262557
S    -2.8443729    0.1616326    1.4822709
C    -3.7819739   -1.3584696    1.7274716
H    -3.0689364   -2.1263779    2.0318295
H    -4.4900373   -1.1565850    2.5340080
H    -4.2742631   -1.6203822    0.7879634
C    -4.1600147    1.2144728    0.8459944
H    -3.7309447    2.2089156    0.7222848
H    -4.5223050    0.7860443   -0.0937525
H    -4.9207630    1.2538663    1.6274545
O    -0.0811278    1.6598055    1.2724100
O    -0.2142052    1.1975760   -1.7104302
S     0.7916586    2.9801244    1.3324842
S    -1.3415260    0.7049031   -2.7510653
C     1.1265501    3.1547242    3.0900453
C    -0.4556918    0.6755116   -4.3160686
H     1.8981047    2.4248969    3.3435948
H     0.2808353   -0.1331076   -4.2781943
H     1.5289506    4.1638051    3.2227662
H    -1.2115524    0.4614398   -5.0761802
H     0.1934237    3.0067232    3.6426228
H     0.0188815    1.6458120   -4.4781512
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O	2.0468349	0.1895874	-0.1262557
S	2.8443729	-0.1616326	-1.4822709
C	3.7819739	1.3584696	-1.7274716
H	3.0689364	2.1263779	-2.0318295
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H	4.2742631	1.6203822	-0.7879634
C	4.1600147	-1.2144728	-0.8459944
H	3.7309447	-2.2089156	-0.7222848
H	4.5223050	-0.7860443	0.0937525
H	4.9207630	-1.2538663	-1.6274545
O	0.0811278	-1.6598055	-1.2724100
O	0.2142052	-1.1975760	1.7104302
S	-0.7916586	-2.9801244	-1.3324842
S	1.3415260	-0.7049031	2.7510653
C	-1.1265501	-3.1547242	-3.0900453
C	0.4556918	-0.6755116	4.3160686
H	-1.8981047	-2.4248969	-3.3435948
H	-0.2808353	0.1331076	4.2781943
H	-1.5289506	-4.1638051	-3.2227662
H	1.2115524	-0.4614398	5.0761802
H	-0.1934237	-3.0067232	-3.6426228
H	-0.0188815	-1.6458120	4.4781512
C	0.4660673	-4.2598105	-1.1429061
C	2.3087649	-2.2067139	2.9808912
H	0.8047517	-4.2230911	-0.1055739
H	2.8671913	-2.3764759	2.0611816
H	1.2811630	-4.0635343	-1.8481204
H	1.6285149	-3.0294877	3.2123111
H	-0.0226945	-5.2186958	-1.3393964
H	3.0077597	-1.9995043	3.7932241
S	4.3529864	0.8446418	2.9769363
O	4.7677389	-0.3590717	2.2557232
O	4.0085477	1.9900196	2.1367110
O	3.3959448	0.5831620	4.0704362
Cl	6.0995127	1.4599428	4.0062146
S	-4.3529864	-0.8446418	-2.9769363
O	-4.7677389	0.3590717	-2.2557232
O	-4.0085477	-1.9900196	-2.1367110
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Cl   -6.0995127   -1.4599428   -4.0062146
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O     3.7829688   -1.0232526   -3.9083281
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Cl    3.8381115   -3.2155584   -5.7145618
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O    -1.5749038    1.8333398    4.6721631
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Cl   -3.8381115    3.2155584    5.7145618

Sn(OTf)4(DMSO)2 TPSS
53
Energy = -5168.350059072
Sn    0.0185242    0.1303188   -0.0421137
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S     3.1713578   -0.8184411    0.4565042
S     0.8653844    3.3266946   -0.0439792
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O     2.7295708   -1.6368818    1.5612156
O     1.4832735    3.8219622    1.1581472
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O     1.6577413    3.0752091   -1.2283715
O    -3.4294080    1.9647301   -0.6670538
O     0.0151415   -0.1593113    2.0149815
S    -1.1034978   -0.8608652    2.8735297
C    -1.2904117    0.3113275    4.2281920
H    -1.7774423    1.1886841    3.8008243
H    -1.9363022   -0.1543424    4.9781208
H    -0.3058486    0.5497235    4.6355539
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O     0.0463020    0.4472633   -2.1094733
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H     1.0242961    1.6725790   -4.4129331
H     2.5185067    0.6817084   -4.6661425
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C    -0.4206508    4.6043318   -0.5443639
C     4.3630425    0.4427036    1.1803697
C     0.4531629   -4.4802044   -0.6621453
F    -5.7322179    0.3026127    0.4362242
F    -4.4138405   -1.3766872    0.9036464
F    -4.6902111   -0.7480372   -1.1723046
F    -0.2143894   -5.6427276   -0.7647966
F     1.2415466   -4.5260774    0.4212613
F     1.2188246   -4.3230215   -1.7566324
F     3.7834847    1.1185779    2.1847787
F     4.7703637    1.3110553    0.2430749
F     5.4345900   -0.2145518    1.6606300
F     0.2200474    5.7572257   -0.8145964
F    -1.0796956    4.2094268   -1.6449623
F    -1.2989011    4.8175419    0.4447316


Sn(OTf)4(DMSO)3 TPSS
63
Energy = -5721.690641379
Sn    0.1408207    0.1731854    0.1494472
O    -1.4380716   -1.2751371   -0.4237556
S    -2.5946842   -1.3841437   -1.4123215
O    -3.8602649   -0.9936308   -0.8352218
O    -2.2448483   -0.9243066   -2.7427861
O     1.2460546   -1.6506652    0.2851352
O     1.1864705    1.9802623   -0.4357923
O    -1.4495024    1.5142818   -0.1777006
S     1.3350993   -2.7147719    1.3865387
S     2.6949257    2.2106343   -0.5338953
S    -1.7073987    2.9229462    0.3913280
O     1.8473961   -2.2000482    2.6409452
O     3.1915213    3.0881292    0.5061874
O    -1.4942588    2.9491890    1.8322869
O     0.1906370   -3.5966294    1.4124580
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O	-0.8326338	-0.2804769	2.0176633
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H	1.0093552	0.0963108	-4.5875776
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O	1.5751841	0.7007884	1.6982337
S	1.5574864	0.8778828	3.2404240
C	1.5278955	2.6745592	3.4600482
H	0.5338368	3.0087589	3.1548919
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H	3.9099751	1.1796118	2.9809624
H	3.4436569	0.8233794	4.6918474
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C	-2.6970374	-3.2562007	-1.5614561
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C	2.7374459	3.2525411	-2.0977889
F	-3.6904402	-3.5726977	-2.4122326
F	-2.9642452	-3.8257243	-0.3675871
F	-1.5497661	-3.7797708	-2.0346252
F	-3.9095083	2.7696070	-1.1200054
F	-4.1840914	2.0438877	0.9248011
F	-4.0123393	4.1865397	0.5392868
F	3.0033469	-4.7607926	1.4660318
F	3.8522768	-2.9835204	0.5183598
F	2.3997748	-4.2084511	-0.5614580
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F	4.0139813	3.6073993	-2.3485847

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Sn(OTf)4(DMSO)4 TPSS
73
Energy = -6275.063020317
Sn   -0.0025326    0.0006444    0.0005927
O    -0.7588582    1.0357599   -1.6276377
O     0.1220266    1.7195272    1.1238860
S    -0.9164584    2.5909771   -1.8667164
S    -0.0317028    1.6505008    2.7330181
C    -2.3059071    2.6130001   -3.0080743
C    -1.1983368    2.9975270    2.9998247
H    -3.1847239    2.3380107   -2.4221777
H    -2.1394539    2.6862951    2.5430265
H    -2.3964659    3.6403080   -3.3738080
H    -1.3039277    3.1012921    4.0805864
H    -2.1049640    1.9025319   -3.8189754
H    -0.8119208    3.9031337    2.5281572
C     0.4373699    2.9943975   -2.9846766
C     1.5152653    2.4349722    3.2226510
H     1.3574951    2.9139974   -2.4021684
H     2.3060409    1.7107886    3.0253089
H     0.4433663    2.3165360   -3.8467401
H     1.6397325    3.3383973    2.6217580
H     0.2818478    4.0341096   -3.2906873
H     1.4395398    2.6389491    4.2908450
O     0.7526806   -1.0350561    1.6286087
O    -0.1264186   -1.7185486   -1.1222554
S     0.9224016   -2.5894601    1.8642236
S     0.0255945   -1.6513464   -2.7317913
C     2.3105674   -2.6045882    3.0070881
C     1.1865777   -3.0036566   -2.9969428
H     3.1887428   -2.3247593    2.4225757
H     2.1287849   -2.6955388   -2.5401934
H     2.4057836   -3.6317358    3.3721597
H     1.2920240   -3.1095354   -4.0775290
H     2.1053786   -1.8953812    3.8180347
H     0.7962844   -3.9068537   -2.5238131
C    -0.4300654   -3.0036276    2.9800569
C    -1.5253395   -2.4304443   -3.2174684
H    -1.3502078   -2.9255716    2.3972008
H    -2.3123192   -1.7002448   -3.0270883
H    -0.4391976   -2.3284334    3.8442195
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S     3.2691041   -0.0623529   -0.2528291
S    -3.2742232    0.0666865    0.2535718
O     3.7258643    0.6856093    0.8946183
O    -3.7309987   -0.6784371   -0.8957739
O     3.3452362   -1.5112614   -0.2378824
O    -3.3498298    1.5156001    0.2420491
O     0.3064747   -1.3804316   -5.3976006
S    -0.2153471   -0.0257078   -5.6769286
O    -1.5193012    0.2381553   -5.0532505
O     0.7618262    1.0538083   -5.5532032
O    -0.3170838    1.3680130    5.3994378
S     0.2219106    0.0198097    5.6769665
O     1.5271430   -0.2284336    5.0493432
O    -0.7423607   -1.0715720    5.5562587
C     0.6090985    0.0988762    7.5102562
C    -4.3133690   -0.5012710    1.7132864
C    -0.5964897   -0.0997969   -7.5115685
C     4.3075311    0.5023944   -1.7143124
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F     0.5153360   -0.3528342   -8.2308091
F    -1.4979165   -1.0717924   -7.7766581
F    -5.5985306   -0.2062963    1.4672660
F    -3.9274725    0.1221878    2.8376601
F    -4.1956606   -1.8295941    1.8882923
F     3.9218077   -0.1242084   -2.8368926
F     5.5929256    0.2089901   -1.4677445
F     4.1888368    1.8302075   -1.8926763
F    -0.5029358    0.3379134    8.2340324
F     1.4991318    1.0826966    7.7710334
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Sn(OTf)4(DMSO)5 TPSS
83
Energy = -6828.411393552
Sn    0.9228098    0.0931435    0.1199831
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S    -0.5098550   -1.6518357    2.5483207
C    -1.2261709   -3.1715948    1.8886451
H    -0.4746279   -3.6341798    1.2463993
H    -1.4342105   -3.8199348    2.7451689
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C    -1.8946296   -1.0659645    3.5247346
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O	1.8762316	0.8257847	1.7992926
O	-0.2168144	1.8216130	-0.0898095
S	3.3604313	1.3555620	1.9423383
S	-1.8049079	1.5738989	-0.2162462
C	3.8342928	0.6547641	3.5300971
C	-2.2389655	2.5986500	-1.6271620
H	3.9873108	-0.4113944	3.3569692
H	-1.7778457	2.1602904	-2.5166221
H	4.7764299	1.1313465	3.8170474
H	-3.3282173	2.5443673	-1.7027264
H	3.0373328	0.8503614	4.2525463
H	-1.8924354	3.6196835	-1.4530383
C	3.1190687	3.0802826	2.4035101
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H	2.4292500	3.1313064	3.2552842
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O	2.4189675	0.9534522	-1.0312366
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C	2.6127235	3.1701411	-2.4321709
H	1.8800444	3.6880569	-1.8106997
H	2.5977448	3.5649172	-3.4482617
H	3.6079340	3.2024309	-1.9839904
C	3.4669482	0.7303034	-3.4265416
H	3.3057707	-0.3478805	-3.4355897
H	4.3881657	0.9856376	-2.8988197
H	3.4259521	1.1340029	-4.4386969
O	-0.0101718	-0.5626988	-1.6311204
S	-0.7077886	-1.9500612	-1.9562460
C	-2.1015403	-1.4279286	-2.9625156
H	-2.8264318	-0.9653184	-2.2884931
H	-2.5288083	-2.3403636	-3.3895082
H	-1.7371204	-0.7424937	-3.7329927
C	0.3601562	-2.6388991	-3.2352198
H	1.3078301	-2.8971879	-2.7580744
H	0.4890950	-1.8969341	-4.0300064
H	-0.1360233	-3.5435761	-3.6001344
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O	3.5439829	-2.3724991	-1.4643092

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O    -4.3354169   -0.2457897    1.5078449
O    -3.5773897   -1.9584284   -0.1117048
O    -4.3229749    0.2580394   -0.9112232
S     0.2848493    1.2341181   -5.2775518
O    -1.0098263    1.3986450   -4.6163771
O     1.2888966    2.2670424   -4.9354175
O     0.8231749   -0.1307485   -5.2708704
S     0.2842523    1.6654848    4.9617172
O     0.6831475    0.2523824    4.9304797
O    -0.8468752    1.9983996    4.0866953
O     1.4039368    2.6148800    4.9258469
C    -0.0646885    1.5836695   -7.0861493
C    -6.1585177   -1.4133338   -0.0152971
C    -0.4170772    1.8901832    6.6859911
C     3.2637698   -3.9177013    0.6958724
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F    -6.3944703   -2.3847386    0.8945037
F    -6.3715116   -1.9345917   -1.2448662
F    -0.8446125    3.1553084    6.8809824
F     0.5097560    1.6121592    7.6287507
F    -1.4702762    1.0603638    6.8830816
F     2.3147290   -4.6550840    0.0854510
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F     2.9835355   -3.8604489    2.0092789

Sn(OTf)4(DMSO)6 TPSS
93
Energy = -7381.760987039
Sn    0.0008057    0.0013706    0.0029297
O    -2.0076118   -0.4357766   -0.1099605
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C    -3.6179621   -2.3485730    0.7208120
H    -2.8230467   -3.0961000    0.7086461
H    -4.3539959   -2.5889376    1.4908082
H    -4.0647266   -2.2249160   -0.2684147
C    -4.2820075    0.3015072    0.9992311
H    -3.9693577    1.2880258    1.3422453
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H    -5.0549673   -0.0752615    1.6709696
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H	2.8312653	3.0980053	-0.7022190
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C	4.2796034	-0.3033146	-1.0031526
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O	0.3106747	-0.9305856	-1.8448193
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S	-0.3981536	-2.1757088	-2.5189007
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H	-0.3760856	-1.7385481	3.9036184
H	-0.9656192	-2.4951530	-4.7751782
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H	0.0952043	-3.3959707	3.3497317
C	0.9993935	-3.2764581	-2.8164934
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H	1.3180275	-3.6575986	-1.8441413

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O     4.7300469   -0.8259056    2.1998802
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O     3.2440420   -0.9197035    4.1676291
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O    -3.7357570   -1.2717770   -3.0906746
O    -3.2434220    0.9034583   -4.1634238
S     3.2110167    0.1206734   -4.4702352
O     1.8695192    0.5255565   -4.9018141
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In(OTCl)3(DMSO)2   TPSS
36
Energy = -4549.689056109
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S     1.6063752    0.0191155    2.6747968
O     2.8721318    1.3406592   -2.6955114
O     1.2048732    0.2484177    4.0378924
O     2.2435968   -1.0037043   -2.1020133
O     2.2867793    1.0601754    1.9352008
Cl    0.5748410    0.2803804   -4.0105451
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O    -0.6054612    2.0962516    0.8430730
S    -0.3122315    3.3526522   -0.0294299
C     1.3722535    3.8450217    0.3967242
H     2.0342365    3.0994891   -0.0451543
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H    -1.0082872    5.5893992    0.4110328
O    -0.4139136   -1.9339425   -0.6177804
S     0.7727739   -2.8858378   -0.2644355
C     0.0265066   -4.0667550    0.8814056
H    -0.1602648   -3.5173863    1.8059434
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C     0.8767772   -3.9140604   -1.7408766
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In(OTCl)3(DMSO)3   TPSS
46
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S    -1.0657277   -2.0119252    2.6503183
S    -1.6272923   -2.0133850   -2.0375800
C    -2.4604802   -1.7164584    3.7582755
C    -3.2247349   -2.7964299   -1.7216051
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H    -3.0708053   -3.6767071   -1.0933260
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H     0.2903676   -1.5822002    4.5821391
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O     0.5428919    0.4452825   -1.8298557
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O     2.1674165   -2.8883229   -1.2740781
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Cl    3.8395473   -2.9525461    1.0321304
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S     0.8723869    3.0838501    1.0588336
O     0.3837924    3.5306953   -0.2337070
O     0.3221751    3.6593744    2.2574450
Cl    2.9148518    3.6049633    1.0740458

In(OTCl)3(DMSO)4   TPSS
56
Energy = -5656.408684940
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S     1.2556996   -2.2365089   -1.4391992
C     2.7030563   -1.7012188   -2.3743346
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C	0.7729930	-3.6404884	-2.4692716
H	-0.1447861	-4.0411807	-2.0381707
H	0.6226012	-3.2950155	-3.4946152
H	1.5733628	-4.3838246	-2.4130845
O	0.1395576	1.8092574	-1.1322938
S	1.7054238	1.7800783	-0.9879238
C	2.2477708	2.6387412	-2.4801209
H	2.0088609	1.9909733	-3.3255035
H	3.3280591	2.7731063	-2.3947057
H	1.7156860	3.5894237	-2.5577755
C	2.0475166	3.0793930	0.2159002
H	1.6289666	2.7396837	1.1634064
H	1.5612023	4.0000731	-0.1135302
H	3.1326136	3.1731635	0.2931346
O	-2.4223380	0.1462111	-1.9897019
S	-3.7816752	0.8949955	-1.9466039
C	-4.8719263	-0.0778545	-0.8788683
H	-5.8872138	0.3054513	-1.0179603
H	-4.5400426	0.0972805	0.1449869
H	-4.7898920	-1.1339497	-1.1454513
C	-4.4819162	0.4228558	-3.5454293
H	-4.4703099	-0.6657175	-3.6327975
H	-3.8557674	0.8826088	-4.3121132
H	-5.4992095	0.8193741	-3.6028061
O	0.5900553	-0.1372825	1.0931090
S	0.4916041	-0.7476188	2.5263475
C	1.6145713	-2.1602700	2.4575382
H	1.7503043	-2.5184346	3.4822743
H	1.1167301	-2.9241749	1.8572551
H	2.5585193	-1.8382805	2.0086346
C	1.4993821	0.3667115	3.5225152
H	2.4741574	0.5047818	3.0457776
H	0.9408501	1.3004780	3.5972922
H	1.6006016	-0.0914103	4.5108880
O	-2.1087629	-1.4823045	0.5672751
S	-2.2475443	-2.9555001	0.2859161
O	-0.9636777	-3.6372930	0.2361120
O	-3.2136712	-3.2500120	-0.7501769
Cl	-3.1303269	-3.5870222	2.0776136
O	4.0683754	-0.8014449	0.4621849
S	5.0090953	0.2887265	0.1948473
O	6.4128215	-0.0555300	0.1349790

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O     4.5369021    1.2562172   -0.8073440
Cl    4.8680978    1.4694208    2.0507120
O    -2.3737959    1.4127657    0.6076047
S    -2.3213710    2.3267231    1.8136420
O    -3.6062951    2.4086504    2.4602724
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Cl   -2.0454330    4.2118486    0.9025550

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S     2.4793038    1.3558842   -2.5738586
C     3.0383643    0.6193166   -4.1296814
H     2.1524711    0.2108153   -4.6190898
H     3.4796430    1.4073429   -4.7459712
H     3.7572904   -0.1733283   -3.9108545
C     4.0938669    1.8515872   -1.9224106
H     3.9037436    2.2858442   -0.9405036
H     4.7320987    0.9683864   -1.8491891
H     4.5116838    2.6055375   -2.5956055
O    -0.6952511    1.2083885   -1.3146685
O    -0.9837514   -0.3585305    1.2495882
S    -2.2232336    0.8836029   -1.3425119
S    -1.1872450   -0.1882851    2.7797253
C    -2.5695315    0.5929979   -3.0926825
C    -2.3142506   -1.5443656    3.1733465
H    -2.0398216   -0.3220699   -3.3614952
H    -1.7347469   -2.4667454    3.0951163
H    -3.6488630    0.4557364   -3.1863098
H    -2.6538916   -1.4028140    4.2035989
H    -2.2074532    1.4425132   -3.6765562
H    -3.1503609   -1.5341377    2.4655674
C    -2.9951531    2.5074763   -1.1854365
C    -2.3385613    1.1926580    2.9470114
H    -2.7336653    2.8811673   -0.1951748
H    -1.7978804    2.0836663    2.6200542
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H    -3.2313733    1.0096724    2.3394972
H    -4.0735051    2.3516159   -1.2623793
H    -2.5872129    1.2713159    4.0102578
O    -0.5212660   -1.5428346   -1.2935026
S    -0.7978778   -2.9732216   -0.7629584
C    -2.5107309   -3.2909103   -1.2351189
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C     0.0218726   -4.0640765   -1.9506739
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H    -0.3390525   -3.8313491   -2.9555612
H    -0.2158040   -5.0959672   -1.6763935
O     1.7220162    0.1089221    1.8600564
S     3.1412635    0.6480103    2.1581114
C     2.8887135    1.8829233    3.4589072
H     2.4405468    2.7625615    2.9928933
H     3.8713963    2.1396336    3.8654962
H     2.2420465    1.4588528    4.2307932
C     3.8835108   -0.6404085    3.1871982
H     4.0375628   -1.5095260    2.5477295
H     3.2085115   -0.8674967    4.0156246
H     4.8441843   -0.2630774    3.5493907
O     1.8369826   -2.0321311    0.0489970
S     3.2319246   -2.4154964   -0.3181368
O     3.3406510   -3.0757858   -1.6029980
O     4.2289058   -1.4142675    0.0229767
Cl    3.5718257   -3.9841385    1.1001218
O     1.5176954    2.1977861    0.0364076
S     0.9377277    3.4804852    0.5503517
O     1.9188297    4.2627547    1.2785801
O    -0.3817746    3.3310047    1.1354273
Cl    0.6246220    4.5893622   -1.2316572
S    -5.1887207   -0.4254019    0.2041324
O    -5.0633775   -0.2340897   -1.2423049
O    -4.5592030   -1.6455840    0.7215224
O    -4.9535569    0.7728853    1.0093440
Cl   -7.2780861   -0.8059088    0.4703664

In(OTCl)3(DMSO)6   TPSS
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S     0.3697121    2.3383658   -1.5486779
C     0.0873484    4.0112760   -0.9438846
H     0.4976709    4.0531058    0.0648448
H     0.6688539    4.6694986   -1.5933070
H    -0.9865085    4.2186349   -0.9629093
C    -0.3604594    2.5173375   -3.1888058
H    -0.3306607    1.5344540   -3.6639727
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H	-1.3909801	2.8696293	-3.0815161
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O	1.5076677	-0.9287576	-0.5294894
O	-1.7613237	-1.3120650	-0.3234971
S	1.6637457	-1.5543738	-1.9512386
S	-2.2269471	-1.2400339	-1.8142822
C	2.9078595	-2.8364471	-1.7289951
C	-3.9397869	-0.6940703	-1.7399259
H	2.4919377	-3.6028191	-1.0689586
H	-3.9654788	0.3280801	-1.3474544
H	3.0903753	-3.2723798	-2.7153547
H	-4.3212904	-0.7053643	-2.7655663
H	3.8147441	-2.3793069	-1.3256261
H	-4.5036445	-1.3792348	-1.1020728
C	2.6697387	-0.3760241	-2.8831447
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H	2.0563099	0.4920089	-3.1246275
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H	-3.2025656	-3.4130863	-1.5595102
H	2.9752760	-0.8828205	-3.8034607
H	-2.8718120	-2.9840470	-3.2766323
O	-0.0349324	-1.6946917	2.0437013
S	-0.3035965	-3.1676196	1.5610889
C	0.6526694	-4.1379548	2.7417487
H	1.7051740	-3.9920758	2.4989230
H	0.3870417	-5.1838913	2.5770956
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C	-1.9582639	-3.5419287	2.1856243
H	-2.6436631	-2.8919942	1.6401706
H	-1.9923732	-3.3375835	3.2579925
H	-2.1527471	-4.5913714	1.9552657
O	-1.5738629	0.8033083	2.0432160
O	1.3851293	1.0443014	1.6374970
S	-1.7386554	2.3414572	2.2289981
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C	-3.4979147	2.5472720	2.5351408
C	3.6025203	2.3177999	2.2636564
H	-4.0089129	2.3082971	1.5963270
H	3.2600685	3.2522709	1.8195467
H	-3.6611300	3.6009233	2.7783501
H	4.6894886	2.2545772	2.1613716
H	-3.7943286	1.8879100	3.3547276
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C	-1.1198060	2.6228537	3.9077125

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C     3.5473748   -0.4127167    2.2035478
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H    -1.6215139    1.9412404    4.5983116
H     3.2579338   -0.3177336    3.2524673
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H     4.6350273   -0.4202897    2.0885471
S    -4.0410404    3.2873201   -1.1433218
O    -3.5432636    3.0012322   -2.4857778
O    -4.5908615    2.1220474   -0.4335023
O    -3.1875860    4.1419187   -0.3166850
Cl   -5.7703668    4.4963774   -1.4876622
S     3.7784499    3.2143568   -1.7131131
S     0.4279665   -5.5799192   -0.6736188
O     2.8624501    3.2741011   -2.8561407
O     0.1927925   -4.7451799   -1.8543665
O     3.1854593    3.6641341   -0.4464374
O     1.6953016   -5.3090094    0.0124277
O     4.5838909    1.9992240   -1.6135191
O    -0.7241052   -5.7312697    0.2216292
Cl    5.2138981    4.7367890   -2.1439201
Cl    0.6912117   -7.5294758   -1.4795668

In(OTf)3(DMSO)2   TPSS
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Energy = -4182.382129843
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O     1.6129516   -0.0229563    1.3345600
O    -1.4853764    0.3895295    2.2284707
S    -2.7805511    0.6304801    1.5120969
O    -3.5152948    1.8234515    1.8414653
O    -2.4986066    0.3773309    0.0578526
S     0.6253949   -0.4277412   -2.9190305
S     2.8333923    0.8939890    1.4814187
O     1.4998944    0.3076697   -3.7997823
O     2.9414901    1.4415569    2.8115311
O     1.0045178   -1.7575848   -2.4732945
O     3.0218970    1.7504367    0.3281330
O    -0.1449442    2.3838322    0.3578415
S    -0.4410872    3.2879568   -0.8734150
C     1.1767658    3.7247516   -1.5483719
H     1.5637596    2.8286929   -2.0357222
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O    -0.3980421   -1.9024691    0.3842273
S     0.8544463   -2.8316836    0.3516434
C     0.8809596   -3.5398918    2.0149360
H     1.1561342   -2.7269215    2.6895058
H     1.6469480   -4.3201932    2.0392914
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C     0.2476686   -4.2554301   -0.5722480
H     0.1348519   -3.9163000   -1.6025396
H    -0.7043985   -4.5802840   -0.1470232
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C    -3.8808009   -0.8002179    2.0336376
C     4.1782996   -0.4113144    1.3633392
C    -0.9713563   -0.6707525   -3.8750129
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F    -4.1279698   -0.7180610    3.3505483
F    -3.2865727   -1.9780812    1.7758284
F     4.0064806   -1.3659413    2.3077441
F     5.3794077    0.1592464    1.5512979
F     4.1696790   -1.0106965    0.1574450
F    -1.8939686   -1.2882201   -3.1088312
F    -1.4735831    0.5105454   -4.2794243
F    -0.7387144   -1.4330103   -4.9590425

In(OTf)3(DMSO)3   TPSS
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O    -0.6196711   -2.2818015   -0.3539466
S    -0.6793584   -1.9567446    2.9014809
S    -1.3556532   -2.7657820   -1.6228008
C    -1.8760529   -1.4682585    4.1623405
C    -2.6345589   -3.8713738   -0.9845914
H    -2.7903345   -1.2050250    3.6278215
H    -3.3165662   -3.2434735   -0.4083478
H    -2.0471597   -2.3256266    4.8198473
H    -3.1458693   -4.3245406   -1.8389025
H    -1.4801046   -0.6103272    4.7106194
H    -2.1682148   -4.6296842   -0.3512506
C     0.7618254   -2.2453027    3.9579572
C    -0.2354584   -3.9997324   -2.3244538
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H    -0.0109207   -4.7543903   -1.5674076
H     0.5566818   -3.1094840    4.5960344
H    -0.7240797   -4.4407748   -3.1981223
O     0.1493034    0.1066658   -2.0427174
S     0.8193288    1.3606251   -2.6827958
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H     2.4922538    0.0690224   -3.7190341
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H    -1.0732534    1.4589473   -4.1558079
H    -0.1278510    2.9993119   -4.1248670
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O    -2.1242047    0.4209411   -0.1090038
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O    -3.3932289   -1.3688734    1.0350858
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S     0.1659370    3.1017531    0.6369373
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O    -0.5246930    3.4394306    1.8570539
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F    -4.3968032   -0.6516530   -1.6849689
F    -4.6563362    1.4618631   -1.1909251
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Energy = -5289.102796825
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H	2.4779107	-2.1661238	-3.3940412
C	0.6309277	-3.9915271	-2.2391653
H	-0.3277042	-4.2503328	-1.7892300
H	0.5348162	-3.7734935	-3.3052857
H	1.3601483	-4.7866967	-2.0600336
O	0.3671173	1.6101559	-1.6601835
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C	2.5455359	1.9052896	-3.1336379
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H	-5.7485755	0.5016374	-1.5790974
H	-4.4823324	0.4742312	-0.3155949
H	-4.7099363	-0.9709718	-1.3733937
C	-4.2722314	0.1495865	-4.0026489
H	-4.3339361	-0.9366940	-3.9078436
H	-3.5964982	0.4326109	-4.8116828
H	-5.2577126	0.5955093	-4.1615431
O	0.6329182	-0.0124071	0.8284885
S	0.4873454	-0.4440571	2.3239510
C	1.5753955	-1.8794121	2.4532373
H	1.6922215	-2.1003883	3.5184757
H	1.0588400	-2.7039001	1.9577634
H	2.5337207	-1.6567422	1.9735013
C	1.5035538	0.7696542	3.1862042
H	2.4796303	0.8321321	2.6943983
H	0.9507108	1.7091557	3.1419099
H	1.5923340	0.4372731	4.2247293
O	-2.1274279	-1.2795896	0.4035351
S	-2.4013705	-2.7604871	0.2774056
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F    -4.4278687   -2.2976521    1.9511808
F    -2.5312167   -2.7397518    2.9456041
F    -2.9359748    4.5376549   -0.1080762
F    -2.4153912    4.9051934    1.9826314
F    -0.8607669    4.3456905    0.5521459
F     7.1914436    1.0765933    0.4730869
F     6.7909470   -0.5937914    1.8248624
F     7.1376749   -0.9670507   -0.3007889

In(OTf)3(DMSO)5   TPSS
75
Energy = -5842.443563646
In    0.8030093    0.0162611   -0.1564822
O     2.2981591    0.1832495   -1.7274796
S     2.8936827    1.4531982   -2.3778237
C     3.5996396    0.7587071   -3.8924324
H     2.7590542    0.4699133   -4.5258758
H     4.1944589    1.5331602   -4.3842904
H     4.2021900   -0.1142669   -3.6322320
C     4.4374934    1.7616069   -1.4831689
H     4.1500039    2.1611523   -0.5100100
H     4.9779240    0.8178042   -1.3816763
H     5.0100873    2.5056226   -2.0442433
O    -0.5520834    1.3330664   -1.2760539
O    -0.8866322   -0.4408003    1.1398011
S    -2.0753792    0.9970595   -1.3552548
S    -1.1307388   -0.3936837    2.6721670
C    -2.3982917    0.8652650   -3.1289557
C    -2.2712414   -1.7718494    2.9237868
H    -1.8502796   -0.0123579   -3.4745018
H    -1.6901540   -2.6873944    2.7934785
H    -3.4745711    0.7215845   -3.2456846
H    -2.6432224   -1.7087842    3.9507743
H    -2.0433006    1.7701783   -3.6277648
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H	-3.0845567	-1.7053174	2.1924728
C	-2.8690081	2.5920350	-1.0627343
C	-2.2804498	0.9763158	2.9201834
H	-2.6156211	2.8822010	-0.0427518
H	-1.7291076	1.8859261	2.6700681
H	-2.4891047	3.3244652	-1.7780756
H	-3.1640840	0.8436149	2.2861034
H	-3.9447865	2.4284151	-1.1563691
H	-2.5465458	0.9773845	3.9822657
O	-0.3935286	-1.3796188	-1.5071765
S	-0.6927124	-2.8574017	-1.1512901
C	-2.4064181	-3.0988688	-1.6642244
H	-3.0510820	-2.5364496	-0.9807023
H	-2.6198178	-4.1692267	-1.5807773
H	-2.5287046	-2.7591600	-2.6956882
C	0.1200947	-3.8048840	-2.4612634
H	1.1938485	-3.6317603	-2.3619446
H	-0.2465295	-3.4565576	-3.4301144
H	-0.1142326	-4.8622655	-2.3083121
O	1.7937618	-0.0221469	1.8839926
S	3.1229287	0.5883156	2.3763770
C	2.6740241	1.4861731	3.8843606
H	2.1327132	2.3813763	3.5767772
H	3.6021140	1.7712016	4.3881501
H	2.0669185	0.8312353	4.5138833
C	3.9867449	-0.7873424	3.1741020
H	4.3060359	-1.4578192	2.3767307
H	3.3066965	-1.2840295	3.8699310
H	4.8541530	-0.3718471	3.6954235
O	1.8946269	-2.0251345	-0.0597150
S	3.2655290	-2.4618948	-0.4780745
O	3.3635441	-2.8745619	-1.8679684
O	4.3380894	-1.6302212	0.0545393
O	1.6374130	2.1981817	0.1386340
S	1.1330698	3.4020975	0.8817506
O	2.1126638	3.9115282	1.8292507
O	-0.2429580	3.2787110	1.3349046
S	-5.0972422	-0.4233086	0.0233102
O	-4.9500949	-0.0998007	-1.4007771
O	-4.4686196	-1.6871163	0.4374919
O	-4.8729563	0.6998453	0.9388789
C	-6.9304568	-0.7793345	0.2018749
C	1.1058273	4.7157857	-0.4602122
C	3.3921953	-4.0729997	0.4796486
F	-7.3061841	-1.8135043	-0.5856844

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F    -7.2399971   -1.1012423    1.4796913
F    -7.6731092    0.2953671   -0.1452483
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F     3.2846061   -3.8656756    1.8135176
F     4.5782351   -4.6652236    0.2452473
F     0.2463170    4.4103134   -1.4522846
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F     2.3377957    4.8581033   -1.0064399

In(OTf)3(DMSO)6   TPSS
85
Energy = -6395.789485595
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S     0.7363273    2.1848324   -0.8895646
C     0.6133555    3.8465032   -0.2048890
H     0.9318873    3.7812086    0.8354380
H     1.3293723    4.4562596   -0.7604063
H    -0.4206286    4.1914966   -0.3004101
C     0.2006109    2.5490601   -2.5731689
H     0.1520017    1.5982472   -3.1083974
H    -0.7828442    3.0280563   -2.5339290
H     0.9738845    3.1859286   -3.0087389
O     1.3593261   -1.2409498   -0.0274157
O    -1.9431810   -1.2142674   -0.0893137
S     1.5606019   -1.7845714   -1.4771063
S    -2.2563390   -0.9966101   -1.6055301
C     2.5875167   -3.2460925   -1.2539474
C    -3.8767749   -0.2155641   -1.6352295
H     2.0078236   -3.9907784   -0.6997884
H    -3.7963516    0.7821200   -1.1897545
H     2.8077474   -3.6318136   -2.2533747
H    -4.1650122   -0.1263015   -2.6873558
H     3.5033905   -2.9542849   -0.7337862
H    -4.5836871   -0.8420021   -1.0853666
C     2.8017302   -0.7031002   -2.2227931
C    -2.7085571   -2.6451202   -2.1771954
H     2.3391616    0.2590874   -2.4441035
H    -1.8344150   -3.2979417   -2.0830570
H     3.6393282   -0.5500284   -1.5378100
H    -3.5387535   -3.0195749   -1.5736628
H     3.1218723   -1.1842753   -3.1519559
H    -3.0033357   -2.5476981   -3.2265384
O    -0.4591603   -1.9602539    2.3554330
S    -0.8698769   -3.3506301    1.7414836
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C	-0.1287982	-4.5117612	2.9038174
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H	-0.3892279	-4.2061413	3.9200489
C	-2.5997964	-3.5530792	2.2252102
H	-3.1561947	-2.7801820	1.6933020
H	-2.6881138	-3.4283119	3.3066774
H	-2.9039764	-4.5479387	1.8940442
O	-1.7042365	0.7077070	2.4113340
O	1.2948797	0.6105010	2.2558784
S	-1.7032511	2.2428384	2.6771510
S	2.8205110	0.3857091	1.9916738
C	-3.4482595	2.6516828	2.8151572
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H	-3.8790149	2.5299099	1.8150755
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H	-3.5098038	3.7033189	3.1082001
H	4.6696437	1.3537117	3.1044769
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C	-1.2422409	2.3569460	4.4251068
C	3.2066010	-1.1350820	2.9005384
H	-0.2016169	2.0357213	4.4962981
H	2.7037802	-1.9476237	2.3746665
H	-1.8933332	1.7071593	5.0144270
H	2.8467718	-1.0523983	3.9285701
H	-1.3386772	3.4015632	4.7341969
H	4.2905545	-1.2768907	2.8669509
S	-3.5319964	3.7147261	-0.8245081
O	-2.9186698	3.4240947	-2.1213156
O	-4.3123772	2.6010646	-0.2541976
O	-2.6712624	4.4014923	0.1449789
S	4.2568088	2.6214201	-0.7480598
S	-0.3069169	-5.7363100	-0.5935700
O	3.4429428	2.8319032	-1.9535695
O	-0.3574817	-4.8211772	-1.7407492
O	3.6366210	3.1215987	0.4901536
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O	4.8806279	1.3008749	-0.6314264
O	-1.5225813	-5.7677576	0.2342739
C	-4.8503516	4.9868842	-1.2268082
C	-0.2726886	-7.4370038	-1.3828572
C	5.7121882	3.7790548	-0.9935653
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F	-5.5255212	5.3539656	-0.1106534

F	-4.3060530	6.1001382	-1.7647727
F	-1.3743714	-7.6432306	-2.1369000
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F	0.8094872	-7.5746549	-2.1810887
F	5.3000690	5.0610310	-1.1186517
F	6.5587721	3.7192872	0.0622577
F	6.4113937	3.4575669	-2.1030891